

SMILES	MP_exp
<chem>CCOC(C[N+](C)(C)C)=O</chem>	162.5
<chem>CCCCCCCCCCCCCCCC[N+](CCCC)(C)C</chem>	83.5
<chem>CCCCCCC(C[N+](CC)(CC)CC)=O</chem>	103
<chem>CCCCCCCCCCCCCCCC[N+](CCO)(CCO)C</chem>	129
<chem>CCCCCCCCCCCCCCCC[N+](c1ccccc1)(C)C</chem>	117
<chem>CCCCCCCC[N+](CCO)(C)C</chem>	117
<chem>CCCCCCCC[N+](CCO)(C)C</chem>	121.5
<chem>CCCCCCCCCCCC[N+](CCO)(C)C</chem>	205.5
<chem>CCCCCCCCCCCCCCCC[N+](CCO)(C)C</chem>	204
<chem>CCCCCCCCCCCCCCCC[N+](CCO)(C)C</chem>	209.5
<chem>CCCCCCCCCCCCCCCC(C[N+](CCO)(C)C)O</chem>	78.5
<chem>CCCCCCCCCCCCCCCC[N+](CC(CO)O)(C)C</chem>	69
<chem>CCCCCCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCCCCCCCCCC)(C)C</chem>	137.5
<chem>CC(CCC[N+](C)(C)C)C</chem>	210
<chem>OCC[N+](C(C)C)(C)C</chem>	275.5
<chem>CCCC[N+](CC)(CC)CC</chem>	213.5
<chem>CCCC[N+](CCCC)(C)C</chem>	166.1
<chem>C[N+](CC(CC)(O)C)(C)C</chem>	168.5
<chem>CCC(C[N+](C)(C)C)OC</chem>	123
<chem>CCOC(C[N+](C)(C)C)CC</chem>	159.5
<chem>CCCC(C[N+](C)(C)C)OC</chem>	102
<chem>CCCCCCCC[N+](C)(C)C</chem>	228.5
<chem>OCCOCC[N+](C)(C)C</chem>	84.5
<chem>CCOC(C[N+](C)(C)C)CC</chem>	148
<chem>CCCC(C[N+](C)(C)C)OC</chem>	99
<chem>CCCC(C[N+](C)(C)C)OCC</chem>	148
<chem>CCCCCCC[N+](CC)(CC)CC</chem>	125.75
<chem>CC(CC[N+](CCC(C)C)(CC)C)C</chem>	127
<chem>CCCC[N+](CCCC)(CCCC)C</chem>	121
<chem>CCOCC[N+](CC)(CC)CC</chem>	97.5
<chem>C#CC[N+](CC)(CC)CC</chem>	199
<chem>CCCC(C[N+](C)(C)C)OCC</chem>	148.5
<chem>CCCCOC(C[N+](C)(C)C)CC</chem>	129
<chem>CCCCOC(C[N+](C)(C)C)CCC</chem>	110.5
<chem>C=CC[N+](CC=C)(CC=C)C</chem>	90
<chem>CCCCCCCC(C[N+](C)(C)C)CC</chem>	226
<chem>CCCCOC(C[N+](C)(C)C)CCC</chem>	106
<chem>CC(CC(C[N+](CC)(CC)C)(O)C)(C)C</chem>	125
<chem>CCOC([N+](C)(C)C)=C</chem>	150.5
<chem>C1CCC(CC([N+](C)(C)C)C)CCC1</chem>	272.5
<chem>C=COCC[N+](CC)(CC)CC</chem>	94.5
<chem>C1CCCC(CC([N+](C)(C)C)C)CCC1</chem>	249
<chem>CC(CC(C[N+](CC(CC(C)C)C)C)(C)C)(C)C</chem>	209.5
<chem>CCCCCCCCCCCC[N+](CCCC)(C)C</chem>	39.95
<chem>C#CC[N+](CC=C)(CC=C)CC=C</chem>	102.5
<chem>CCCC[N+](CC(C=C)O)(C)C</chem>	79
<chem>c1ccc(C[N+](CC=C)(C)C)cc1</chem>	99.5
<chem>CCCC[N+](CC=C)(CC#C)CC#C</chem>	89
<chem>c1cc(c(C[N+](C)(C)C)cc1)C</chem>	213.5
<chem>C=CC[N+](c1ccccc1)(C)C</chem>	125.5
<chem>CCCC(OCC[N+](C)(C)C)=O</chem>	100.5
<chem>c1ccc(CCCC[N+](C)(C)C)cc1</chem>	182
<chem>c1ccc(CCCCC[N+](C)(C)C)cc1</chem>	164.5

c1ccc(C[N+](CCC)(C)C)cc1	139.5
COc1ccc(C[N+](C)(C)C)cc1	148.75
CCCCCCCCCCCCCCCC[N+](CC)(CC)CC	183
CCCCCCCCCCCCCCCC[N+](CCCC)(CCCC)C	51
c1ccc(C[N+](CCO)(C)C)cc1	130.5
c1ccc(C(C[N+](CC)(CC)C)O)cc1	155
CCCCCCCC[N+](CC(O)=O)(C)C	155.5
c1ccc([N+](CC=C)(CC=C)CC#C)cc1	137.5
c1ccc(C[N+](CCC)(CCC)CCC)cc1	187.75
c1ccc(C([N+](CC)(CC)C)CO)cc1	153
CCCCCCCCCCCCCCCC[N+](C1CCCC1)(C)C	140.5
c1cc(c(C[N+](c2ccccc2)(C)C)cc1)C	87.5
c1ccc(C[N+](Cc2ccccc2)(CC)CC)cc1	147
c1ccc(C[N+](c2ccc(cc2)CC)(C)C)cc1	158.5
CCCCCCCCCCCC[N+](CCOC(=O)C)(C)C	64.5
CC=Cc1ccc([N+](Cc2ccccc2)(C)C)cc1	104.5
CCCCC[N+](c1c(cccc1)OC)(C)C	181.5
c1ccc(C(C[N+](CC2CCCC2)(C)C)=O)cc1	186
COc1ccc([N+](Cc2ccccc2)(CC=C)C)cc1	147.5
c1ccc(C(OC(c2ccccc2)[N+](C)(C)C)=O)cc1	136.5
O=C(CCCCCCCCC[N+](CCCCCCCC)(C)C)O	109.5
c1ccc(CCC[N+](CC(c2ccccc2)=O)(C)C)cc1	124.5
CCCCCCCCCCCCCCCC[N+](CC(OCC)=O)(C)C	62
CCCCCCCCCCCCCCCC[N+](CCOC(=O)C)(C)C	84
CCCCCOCc1ccc([N+](Cc2ccccc2)(C)C)cc1	89.5
CCCCCCCCc1ccc([N+](Cc2ccccc2)(C)C)cc1	87.5
CCCCCCCCCCCCCCCC[N+](Cc1ccccc1)(C)C	49
COc1cc(C[N+](CC(c2ccccc2)=O)(C)C)ccc1	151
CCCCCCCCCCCCCCCC[N+](CCOC(=O)C)(CC)CC	70.5
CCCCCCCCCCCCCCCC[N+](CCCCC(OC)=O)(C)C	67
CCCCCCCCCCCCCCCC[N+](Cc1ccccc1)(C)C	60
c1ccc(OC[C[N+](CCOCc2ccccc2)(CC)CC)cc1	78.25
CCCCCCCCCCCCCCCC[N+](CCCCCCCC(OC)=O)(C)C	60
CCCCCCCCCCCCCc1ccc([N+](Cc2ccccc2)(C)C)cc1	86.5
CCCCCCCCCCCCCCCC[N+](CCOC(=O)C)(CCCC)CCCC	53
CCCCCCCCCCCCCOc1c([N+](CCCCCCCC)(C)C)cccc1	39.25
CCCCCCCCCCCCCOc1c([N+](CCCCCCCCCCCC)(C)C)cccc1	44.25
CCCCCCCCCCCCCCCC[N+](c1c(cccc1)OCCCCCCCCCCCC)(C)C	46.75
c1ccc(CC[N+](C)(C)C)cc1	238.5
C[N+](O)(C)C	246
CCCC([N+](C)(C)C)C	227.25
C1CC([N+](C)(C)C)CC1	281
C=CC[N+](C)(C)(C)(C)C	247.5
C1CC([N+](C)(C)C)CO1	250
C1CCC([N+](C)(C)C)CCC1	277.5
Cc1cc(c(cc1C)C[N+](C)(C)C)C	253.75
CCCCCCCCCCCC[N+](CCO)(CCO)CC	70
C[N+](Cc1c2c(c(cc1)C)cccc2)(C)C	233
CCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCC)(C)C	50.5
CCCCCCCCCCCCCCCC[N+](CCCCCCCC)(C)C	60.5
c1ccc(C[N+](C(C(OC)=O)CCCC)(C)C)cc1	146.5
c1ccc(OCCCC[N+](Cc2ccccc2)(C)C)cc1	129
CC[N+](CCOC(C(c1ccccc1)CCC)=O)(CC)C	90
c1ccc(C[N+](C(C(OC)=O)CCCC)(C)C)cc1	117.5

c1ccc(Oc2cc(C[N+](c3ccccc3)(C)C)ccc2)cc1	126.5
CCCCC[N+](Cc1ccccc1)(CCCCC)CCCCC	102
c1ccc(OCCCC[N+](Cc2ccccc2)(C)C)cc1	139.75
CC(c1cc(C[N+](Cc2c(ccc(c2)C(C)C)(C)C)c(cc1)C)C	225.75
CC[N+](CCOC(C(c1ccccc1)CCCC)=O)(CC)C	78
CC(c1cc(C[N+](Cc2ccccc2)(Cc3ccccc3)C)c(cc1)C)C	206.5
c1ccc(C[N+](CCCCOc2c3c(ccc2)cccc3)(C)C)cc1	140
c1cc2c(cc(OCCCC[N+](Cc3ccccc3)(C)C)cc2)cc1	161.5
CCCCCC[N+](C)(C)C	182.5
C=CC[N+](/C=C(\C)C)(C)C	63.5
C1COC([N+](CC)(C)C)CC1	83.5
CC#CC[N+](CC)(CC)CC	117
Cc1cc(C[N+](C)(C)C)cc(c1)C	238.75
c1ccc(C#CC[N+](CC#C)(C)C)cc1	171.5
c1ccc(C[N+](/C=C(\C)C)(C)C)cc1	165
COc1ccc(CC[N+](C)(C)C)cc1	217.95
CCCCCCCCCCCCCCCC[N+](CCCCCCCC)(C)C	57.5
c1ccc(CC[N+](c2ccccc2)(C)C)cc1	169.5
c1ccc(C([N+](c2ccccc2)(C)C)C)cc1	130.5
Cc1c(c(C[N+](CCO)(C)C)ccc1)C	147.5
c1cc(c(C[N+](CCCO)(C)C)cc1)C	128.5
CC(OCC[N+](Cc1ccccc1)(C)C)=O	126
Cc1c(c(C[N+](CCCO)(C)C)ccc1)C	169.75
CCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCC)(C)C	62.5
c1ccc(C[N+](C(C(OCC)=O)C)(C)C)cc1	117.5
c1ccc(Oc2cc(C[N+](CC)(CC)CC)ccc2)cc1	161.5
CCCCCCCCCCCC[N+](Cc1c(ccc(c1)C(C)C)(C)C	153.5
CCCCCCCCCCCC[N+](CCc1c(ccc(c1)C(C)C)(C)C	113.5
CC[N+](CCOC(C(c1ccccc1)(CC(C)C)CC)=O)(CC)C	143
CCCCCCCCCCCC[N+](CCC)(CC)CC	97.5
CCCCCCCCCCCC[N+](COCC)(CC)C	175.5
O=C(CC[N+](CC(O)=O)(C)C)O	150.5
CCCCCCCCCCCC[N+](CC(O)=O)(CC)C	102.5
CCCCCCCCCCCC[N+](Cc1ccccc1)(CC)C	104
CCCCCCCCCCCC[N+](Cc1ccccc1)(CCCC)C	77.5
Oc1ccc(C[N+](C)(C)C)cc1	165.5
CCCCCCCCCCCCCCCC[N+](Cc1ccc(cc1)O)(C)C	129
CC(C[N+](Cc1c(cccc1)C)(C)C)=O	123
Cc1ccc(C[N+](CC(OC)=O)(C)C)cc1	117
COC(C[N+](Cc1c(cccc1)C)(C)C)=O	131.5
CC(CC(C[N+](C)(C)C)=O)C	134
CCOC(C[N+](C)(C)C)OCC	151
OCC(C[N+](C)(C)C)O	120.5
c1ccc(C#CC[N+](CC)(CC)CC)cc1	156.5
C=CC[N+](c1c(ccc(c1)C)O)(C)C	151
COc1cc(C[N+](C)(C)C)cc(c1)OC	194
Cc1cc([N+](CC=C)(C)C)c(c(c1)C)O	106
C=C(C[N+](c1c(ccc(c1)C)O)(C)C)C	152.5
c1ccc(C[N+](c2ccc(cc2)OC)(C)C)cc1	129
c1ccc(C(C([N+](CC#C)(C)C)c2ccccc2)=O)cc1	150.5
c1ccc(/C=C/C[N+](c2c(ccc(c2)C)O)(C)C)cc1	151.5
COC(C[N+](Cc1c2c(ccc1)cccc2)(C)C)=O	162
CCCCCCCCCCCC[N+](Cc1ccc(cc1)C(c2ccccc2)=O)(C)C	125.5
O=Cc1ccc([N+](C)(C)C)cc1	209

c1ccc(/C=C/C[N+](C/C(=C\C=C)C)(C)C)cc1	159
c1ccc(C#CC[N+](C/C=C/c2ccccc2)(C)C)cc1	145.5
c1ccc(C(C[N+](C@H)(c2ccccc2)C)(C)C=O)cc1	126.5
O=Cc1ccc(OCCCCCCCCC[N+](C)(C)C)cc1	117.5
C#CC[N+](CC#Cc1c2c(ccc1)cccc2)(C)C	141.5
C#CC[N+](CC#Cc1c2c(ccc1)cccc2)(CC)CC	125.5
OCCC[N+](CC)(CC)CC	166
CCCCCCCCC[N+](CC)(CC)CC	106.5
Oc1cc([N+](C)(C)C)ccc1	207
c1ccc(C(C[N+](C)(C)C)C)cc1	179
CCCCCCCCCCCCC[N+](C(O)C)(C)C	116.5
c1ccc(C(C[N+](C)(C)C)C(C)C)cc1	170.5
C=C(C[N+](c1cc(ccc1)O)(C)C)C	113.5
Oc1ccc(C(CC[N+](C)(C)C)=O)cc1	206.5
C[N+](CCC(c1cc(ccc1)OC)=O)(C)C	144
Cc1ccc(C(c2ccc(cc2)C)C[N+](C)(C)C)cc1	246
Cc1ccc([N+](C(c2ccccc2)C)(C)C)cc1	101.5
COc1ccc([N+](C(c2ccccc2)C)(C)C)cc1	108
C=C(C[N+](c1cc(c(c(c1)C(C)(C)C)O)C(C)(C)C)(C)C)C	142
C/C(=C/C[N+](c1cc(c(c(c1)C(C)(C)C)O)C(C)(C)C)(C)C)C	135.5
COc1ccc(C(c2ccc(cc2)OC)C[N+](C)(C)C)cc1	229.25
C=C(C#CC[N+](c1cc(c(c(c1)C(C)(C)C)O)C(C)(C)C)(C)C)C	150
c1ccc(C[N+](c2cc(c(c(c2)C(C)(C)C)O)C(C)(C)C)(C)C)cc1	172.5
CCCCCCCCCCCCC[N+](Cc1c(cccc1)O)(C)C	50.5
c1ccc(/C=C/C[N+](c2cc(c(c(C(C)(C)C)c2)O)C(C)(C)C)(C)C)cc1	159.5
CCCCCCCCCCCC(OCC[N+](CCOC(CCCCCCCCCC)=O)(CC=C)C)=O	77.5
CCCCCCCCCCCC(OCC[N+](CCOC(CCCCCCCCCC)=O)(CC=C)C)=O	88.5
c1ccc(C([N+](CC)(CC)C)C)cc1	153
c1ccc(C([N+](CC)(CC)CC)C)cc1	149
c1ccc(C([N+](CCC)(CCC)CC)C)cc1	161.5
c1ccc(C[N+](C(c2ccccc2)C)(C)C)cc1	154.5
c1ccc(C[N+](C(c2ccccc2)C)(CC)CC)cc1	141.5
C=CCC=CC[N+](Cc1ccccc1)(C)C	124.5
c1ccc(C[N+](C(CC=C)(C=C)C)(C)C)cc1	136
COCC[N+](Cc1ccccc1)(C)C	124.5
OCCC[N+](Cc1ccccc1)(C)C	100.5
C/C=C/C([N+](C)(C)C)C	171.35
CC(OC(C[N+](C)(C)C)C)=O	148.75
c1ccc(C[N@+](c2ccccc2)(CC)C)cc1	155.5
Oc1c(cc(C(C[N+](C)(C)C)O)cc1)O	196
O=C(CCCCC[N+](C)(C)C)O	186
CCCCOC[N+](C)(C)C	73.5
c1ccc(C[N+](CCC)(CC)C)cc1	122.5
c1ccc(C(C[N+](CC(=O)C)(C)C)=O)cc1	151
CC(C[N+](CC(c1ccc(cc1)OC)=O)(C)C)=O	145.5
Oc1c(cc(C[N+](c2ccccc2)(C)C)cc1)C	131.5