

Typical Product Specifications & Properties

(1S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one

CAS Number: : 4695-62-9

Specifications	Limits
Molecular weight	152.23
EINECS	232-107-5
SMILES	<chem>C[C@]12CC[C@H](C1)C(C)(C)C2=O</chem>
InChI	LHXDLQBQYFFVNW-XCBNKYQSSA-N
InChIKey	1S/C10H16O/c1-9(2)7-4-5-10(3,6-7)8(9)11/h7H,4-6H2,1-3H3/t7-,10+/m1/s1
Melting Point	6.1 ° C
Water solubility	2150 mg/L
log P (octanol-water)	3.040
Atmospheric OH Rate Constant	1.19E-11 cm ³ /molecule-sec
Molecular weight	734.04
EINECS	220-153-9
SMILES	<chem>C([C@@H](COC(CCCCCCCCCCCCCC)=O)OC(CCCCCCCCCCCCCC)=O)OP(OCC[N+](C)(C)C)(=O)[O-]</chem>

Specifications	Limits
InChI	KILNVBDSWZSGLL-UHFFFAOYSA-N
InChIKey	1S/C40H80NO8P/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-32-39(42)46-36-38(37-48-50(44,45)47-35-34-41(3,4)5)49-40(43)33-31-29-27-25-23-21-19-17-15-13-11-9-7-2/h38H,6-37H2,1-5H3
Molecular weight	734.04
EINECS	220-530-8
SMILES	<chem>C([C@@H](COC(CCCCCCCCCCCCCC)=O)OC(CCCCCCCCCCCCCC)=O)OP(OCC[N+](C)(C)C)(=O)[O-]</chem>
InChI	KILNVBDSWZSGLL-UHFFFAOYSA-N
InChIKey	1S/C40H80NO8P/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-32-39(42)46-36-38(37-48-50(44,45)47-35-34-41(3,4)5)49-40(43)33-31-29-27-25-23-21-19-17-15-13-11-9-7-2/h38H,6-37H2,1-5H3