Typical Product Specifications & Properties

Propyl Oleate, Sulphated

CAS Number: : 68954-62-1

Specifications	Limits
Molecular weight	303.35
EINECS	200-090-3
SMILES	CN1[C@@H]2C[C@H](C[C@H]1[C@H]3[C@@H]2O3)OC(=O)[C@H](CO)c4ccccc4
InChI	1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-2-4-6-10/h2-6,11-16,19H,7-9H2,1H3/t11-,12?,13?,14?,15-,16+
InChIKey	STECJAGHUSJQJN-MBBCWDQXSA-N
Vapor Pressure	7.18E-09 mm Hg
Water solubility	1.00E+05 mg/L
pKa Dissociation Constant	7.75
Atmospheric OH Rate Constant	5.97E-11 cm3/molecule-sec
log P (octanol-water)	0.98
Henry's Law Constant	3.36E-16 atm-m3/mole
Melting Point	59 ° C

Specifications	Limits
Molecular weight	398.29
EINECS	205-844-5
SMILES	[Br-].C[N+]1(C)[C@@H]2CC(C[C@H]1[C@@H]3O[C@H]23)OC(=O)[C@H](CO)c4ccccc4
InChI	CXYRUNPLKGGUJF-RAFJPFSSSA-M
InChIKey	1S/C18H24NO4.BrH/c1-19(2)14-8-12(9-15(19)17-16(14)23-17)22-18(21)13(10-20)11-6-4-3-5-7-11;/h3-7,12-17,20H,8-10H2,1-2H3;1H/q+1;/p-1/t12-,13-,14-,15+,16-,17+;/m1./s1
log P (octanol-water)	-2.580
Atmospheric OH Rate Constant	5.50E-11 cm3/molecule-sec
Molecular weight	361.30
EINECS	200-747-4
SMILES	[N+](CCOC(=O)CCC(=O)OCC[N+](C)(C)C)(C)(C)C.[ClH-].[ClH-]

Specifications	Limits
InChI	YOEWQQVKRJEPAE-UHFFFAOYSA-L
InChIKey	1S/C14H30N2O4.2ClH/c1-15(2,3)9-11-19-13(17)7-8-14(18)20-12-10-16(4,5)6;;/h7-12H2,1-6H3;2*1H/q+2;;/p-2

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Specifications	Limits
log P (octanol-water)	0.32
Atmospheric OH Rate Constant	2.82E-11 cm3/molecule-sec
pKa Dissociation Constant	6.7
Vapor Pressure	5.65E-10 mm Hg

Specifications	Limits

Atmospheric OH Rate Constant	3.33E-11 cm3/molecule-sec
Storage Temperature	2-8°C
log P (octanol-water)	-7.940
Form	Crystalline Powder
Melting Point	190 ° C
Merck	13,9004
Water solubility	5.00E+05 mg/L
Color	White to yellow
Molecular weight	214.25
Stability	Stable. Combustible. Incompatible with strong oxidizing agents.
EINECS	200-345-9
Storage Temperature	Refrigerator
SMILES	c1cc(ccc1N)S(=O)(=O)NC(=N)N
Melting Point	164 °C
InChI	1S/C7H10N4O2S/c8-5-1-3-6(4-2-5)14(12,13)11-7(9)10/h1-4H,8H2,(H4,9,10,11)
Merck	8875
Molecular weight	214.25
EINECS	200-345-9

Specifications	Limits

InChIKey	1S/C7H10N4O2S/c8-5-1-3-6(4-2-5)14(12,13)11-7(9)10/h1-4H,8H2,(H4,9,10,11)
InChI	BRBKORJOKNSWSG-UHFFFAOYSA-N
Atmospheric OH Rate Constant	4.40E-11 cm3/molecule-sec

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pKa Dissociation Constant	11.25
Vapor Pressure	1.47E-07 mm Hg
Melting Point	191.5 ° C
Water solubility	2200 mg/L
log P (octanol-water)	-1.22E+00
Henry's Law Constant	1.01E-15 atm-m3/mole
Solubility	1 M HCl: soluble50mg/mL
Merck	8908
Stability	Stable. Incompatible with strong oxidizing agents.
Water solubility	1g/1000mL at 25 °C

Specifications	Limits
Melting Point	190-193°C
Storage Temperature	-20°C
Color	white to off-white
Form	Powder
Molecular weight	267.30
EINECS	204-858-9
SMILES	Cc1c(noc1NS(=O)(=O)c2ccc(cc2)N)C
InChI	1S/C11H13N3O3S/c1-7-8(2)13-17-11(7)14-18(15,16)10-5-3-9(12)4-6-10/h3-6,14H,12H2,1-2H3
InChIKey	NHUHCSRWZMLRLA-UHFFFAOYSA-N
Stability	Stable. Incompatible with strong oxidizin
Water solubility	<0.1 g/100 mL at 22.5 ºC
Merck	13,9041

Specifications	Limits
InChIKey	BRBKOPJOKNSWSG-UHFFFAOYSA-N
Atmospheric OH Rate Constant	3.24E-11 cm3/molecule-sec

Specifications	Limits
Melting Point	195°C
Storage Temperature	2-8°C
Vapor Pressure	5.08E-08 mm Hg
Melting Point	191 ° C
Water solubility	300 mg/L
log P (octanol-water)	1.01
Henry's Law Constant	1.06E-12 atm-m3/mole
Solubility	acetone: complete50 mg/mL
Molecular weight	361.30
EINECS	200-747-4
SMILES	[N+](CCOC(=O)CCC(=O)OCC[N+](C)(C)C)(C)(C)C.[Cl-].[Cl-]

Specifications	Limits
InChI	YOEWQQVKRJEPAE-UHFFFAOYSA-L
InChIKey	1S/C14H30N2O4.2ClH/c1-15(2,3)9-11-19-13(17)7-8-14(18)20-12-10-16(4,5)6;;/h7-12H2,1-6H3;2*1H/q+2;;/p-2
Atmospheric OH Rate Constant	3.33E-11 cm3/molecule-sec
log P (octanol-water)	-7.940
Melting Point	190 ° C
Water solubility	5.00E+05 mg/L
Stability	Stable. Combustible. Incompatible with strong oxidizing agents.

Specifications	Limits
Storage Temperature	Refrigerator
Melting Point	164 °C
Merck	8875

Specifications	Limits
Melting Point	190-193°C
Storage Temperature	-20°C
Color	white to off-white
Form	Powder

Specifications	Limits
Molecular weight	280.30
EINECS	201-272-5
SMILES	c1(S(=O)(=O)Nc2ccc(nn2)OC)ccc(cc1)N
InChI	1S/C11H12N4O3S/c1-18-11-7-6-10(13-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H,12H2,1H3,(H,13,15)
InChIKey	VLYWMPOKSSWJAL-UHFFFAOYSA-N
Henry's Law Constant	2.37E-14 atm-m3/mole
Melting Point	182.5 ° C
Water solubility	147 mg/L