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Typical Product Specifications & Properties

Ammelide

CAS Number: : 645-93-2

Specifications	Limits
Molecular weight	128.09
InChI	1S/C3H4N4O2/c4-1-5-2(8)7-3(9)6-1/h(H4,4,5,6,7,8,9)
InChIKey	YSKUZVBSHIWEFK-UHFFFAOYSA-N
Molecular weight	830.82
SMILES	[Na+].[Na+].Cc1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)N=Nc3ccc(cc3C)c4ccc(N=Nc5c(O)ccc6cc(=O)[O-]S(=O)(=O)[O-])c(C)c4
InChI	HNBQFKZSMFFZQYWEUAPPMUSA-L
InChIKey	1S/C37H30N4O10S3.2Na/c1-22-4-13-30(14-5-22)54(49,50)51-29 29)38-39-32-15-6-25(18-23(32)2)26-7-16-33(24(3)19-26)40-41-37-20-31(52(43,44)45)21-35(36(27)37)53(46,47)48;;/h4-21,42H,1-31(H,46,47,48);;/q;2*+1/p-2/b3
Vapor Pressure	3.46E-35 mm Hg
Henry's Law Constant	5.08E-31 atm-m ³ /mole
Atmospheric OH Rate Constant	1.82E-11 cm ³ /molecule-sec
Water solubility	2.52E-06 mg/L
log P (octanol-water)	7.860

ISO 9001



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