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Typical Product Specifications & Properties

2-Ethylhexanal dimethylacetal

CAS Number: : 14250-95-4

Specifications	Limits
Molecular weight	174.28
EINECS	238-126-5
SMILES	<chem>C([C@@H](CC)CCCC)(OC)OC</chem>
InChI	PNCLVYKEOAAKCK-UHFFFAOYSA-N
InChIKey	1S/C10H22O2/c1-5-7-8-9(6-2)10(11-3)12-4/h9-10H,5-8H2,1-4H3
Molecular weight	256.34
EINECS	205-547-0
SMILES	<chem>C(CNC(=S)[S-])NC(=S)[S-].[Na+].[Na+]</chem>
InChI	UQJQVUOTMVCFHX-UHFFFAOYSA-L
InChIKey	1S/C4H8N2S4.2Na/c7-3(8)5-1-2-6-4(9)10;;/h1-2H2,(H2,5,7,8)(H2,6,9,10);;/q;2*+1/p-2
log P (octanol-water)	-4.240
Vapor Pressure	9.48E-13 mm Hg





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Specifications	Limits
Henry's Law Constant	1.60E-18 atm-m ³ /mole
Atmospheric OH Rate Constant	1.47E-10 cm ³ /molecule-sec
Water solubility	2.00E+05 mg/L
Molecular weight	388.20
EINECS	215-811-7
SMILES	<chem>c1cc(c(cc1[N+](=O)[O-])Cl)NC(=O)c2cc(ccc2O)Cl.C(CO)N</chem>
InChI	XYCDHXSQODHSLG-UHFFFAOYSA-N
InChIKey	1S/C13H8Cl2N2O4.C2H7NO/c14-7-1-4-12(18)9(5-7)13(19)16-11-3-2-8(17(20)21)6-10(11)15;3-1-2-4/h1-6,18H,(H,16,19);4H,1-3H2
Stability	Stable. Hydrolyzes in concentrated acidic or basic solutions.
Water solubility	100 mg/L
Vapor Pressure	1.00E-14 mm Hg
Melting Point	216 ° C



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Specifications	Limits
Atmospheric OH Rate Constant	2.10E-11 cm ³ /molecule-sec
log P (octanol-water)	0.680
Henry's Law Constant	4.30E-20 atm-m ³ /mole
Chemical Structure	 39267_39267_2-ethylhexanal-dimethylacetal.png chemical structure



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