

## Typical Product Specifications & Properties

# Diethylsafranine

CAS Number: : 4569-86-2

Specifications	Limits
Molecular weight	378.90
Melting Point	285 &deg;C (dec.)
Molecular weight	268.35
EINECS	200-278-5
SMILES	<chem>C(=C(\c1ccc(O)cc1)CC)(\c1ccc(O)cc1)CC</chem>
InChI	1S/C18H20O2/c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11-16(20)12-8-14/h5-12,19-20H,3-4H2,1-2H3/b18-17+
InChIKey	RGLYKWWBQGJZGM-ISLYRVAYSA-N
Melting Point	170.5 &deg; C
Henry's Law Constant	5.80E-12 atm-m <sup>3</sup> /mole
log P (octanol-water)	5.07
Atmospheric OH Rate Constant	1.75E-10 cm <sup>3</sup> /molecule-sec
Vapor Pressure	1.41E-08 mm Hg

Specifications	Limits
Water solubility	12 mg/L
Storage Temperature	0-6&deg;C
Merck	13,3155
Melting Point	170-172 &deg;C
Stability	Isomerizes rapidly in Benzene, Chloroform, and Ether. Keep Shielded from light.
Water solubility	PRACTICALLY INSOLUBLE
Solubility	methanol: 0.1 g/mL, clear, faintly yellow
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