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Typical Product Specifications & Properties

CHLOROFORM-D

CAS Number: : 865-49-6

Specifications	Limits
Molecular weight	380.44
EINECS	201-635-8
SMILES	<chem>c12c(\N=N\c3c(cc(\N=N\c4c(cccc4)C)cc3)C)c(ccc1cccc2</chem>
InChI	1S/C24H20N4O/c1-16-7-3-6-10-21(16)26-25-19-12-13-22(17(2)15 19)27-28-24-20-9-5-4-8-18(20)11-14-23(24)29/h3-15,29H,1-2H3
InChIKey	RCTGMCJBQGBLKT-UHFFFAOYSA-N
log P (octanol- water)	8.720
Melting Point	186 dec ° C
Atmospheric OH Rate Constant	2.01E-11 cm3/molecule-sec
Molecular weight	303.83
EINECS	219-567-2
SMILES	<chem>C(c1ccc(N(C)C)cc1)(c1ccc(N(C)C)cc1)=N.Cl</chem>
InChI	1S/C17H21N3.ClH/c1-19(2)15-9-5-13(6-10-15)17(18)14-7-11-16(8-14)20(3)4;/h5-12,18H,1-4H3;1H



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Specifications	Limits
InChIKey	KSCQDDRPFHTIRL-UHFFFAOYSA-N
Water solubility	Soluble in water or ethanol
Stability	Stable. Incompatible with strong oxidizing agents.
Colour Index	41000
Storage Temperature	Store at room temperature.
Melting Point	>250 °C (dec.)
Atmospheric OH Rate Constant	2.05E-10 cm ³ /molecule-sec
log P (octanol-water)	2.980
Water solubility	1.00E+04 mg/L
Henry's Law Constant	3.64E-09 atm-m ³ /mole
Vapor Pressure	1.29E-06 mm Hg
Molecular weight	250.25



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Specifications	Limits
SMILES	<chem>c1cc(ccc1Cc2ccc(cc2)N=C=O)N=C=O</chem>

Specifications	Limits
InChI	1S/C15H10N2O2/c18-10-16-14-5-1-12(2-6-14)9-13-3-7-15(8-4-13)17-11-19/h1-8H,9H2
InChIKey	UPMLOUAZCHDJJD-UHFFFAOYSA-N
Flash Point	196 °C
Boiling Point	392 °C
Density	1.19
Melting Point	38-44 °C
BRN Number	797662
Water solubility	decomposes
Stability	Stable. Combustible. Incompatible with strong oxidizing agents. Reacts violently with alcohols.
Sensitive	Moisture Sensitive/Lachrymatory
Freezing Point	37?



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Specifications	Limits
Storage Temperature	Refrigerator
Freezing Point	37?
Vapor Pressure	5.00E-06 mm Hg
Henry's Law Constant	8.95E-07 atm-m ³ /mole
Melting Point	38 ° C
log P (octanol-water)	5.220
Water solubility	0.829 mg/L
Atmospheric OH Rate Constant	1.20E-11 cm ³ /molecule-sec
Freezing Point	37?
Molecular weight	120.38
InChI	1S/CHCl3/c2-1(3)4/h1H/i1D
InChIKey	HEDRZ PFGACZZ DS-MICDWDOJSA-N



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Specifications	Limits
Molecular weight	340.41
InChI	1S/C21H24O4/c1-21(2,15-3-7-17(8-4-15)22-11-19-13-24-19)16-5-9-18(10-6-16)23-12-20-14-25-20/h3-10,19-20H,11-14H2,1-2H3
InChIKey	LCFVJGUPQDGYKZ-UHFFFAOYSA-N
Storage Temperature	2-8°C
Water solubility	Soluble in 100% ethanol, dimethyl sulfoxide (100 mM), dimethyl formamide, chloroform, methanol, and ethanol (50 mM). Insoluble in water.
Melting Point	40-44 °C
Refractive Index	1.5735
BRN Number	299026
Boiling Point	210 °C / 1mmHg
Specifications	Limits
Density	1,17 g/cm3



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