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Typical Product Specifications & Properties

Paraquat

CAS Number: : 4685-14-7

Specifications	Limits
Molecular weight	186.25
EINECS	225-141-7
SMILES	<chem>C[n+]1ccc(cc1)c2cc[n+](cc2)C</chem>
InChI	INFDPQAKFNIJBF-UHFFFAOYSA-N
InChIKey	1S/C12H14N2/c1-13-7-3-11(4-8-13)12-5-9-14(2)10-6-12/h3-10H,1-2H3/q+2
Atmospheric OH Rate Constant	2.12E-11 cm ³ /molecule-sec
Melting Point	300 dec ° C
Water solubility	6.20E+05 mg/L
log P (octanol-water)	-4.22E+00
Henry's Law Constant	1.00E-09 atm-m ³ /mole
Vapor Pressure	1.00E-07 mm Hg
Molecular weight	266.34





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Specifications	Limits
EINECS	201-778-6
SMILES	<chem>c1(c(c(c(Cl)c(c1Cl)Cl)Cl)Cl)O</chem>
InChI	1S/C6HCl5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H
InChIKey	IZUPBVBPLAPZRR-UHFFFAOYSA-N
Vapor Pressure	1.10E-04 mm Hg
pKa Dissociation Constant	4.7
Atmospheric OH Rate Constant	5.50E-13 cm ³ /molecule-sec
Water solubility	14 mg/L
log P (octanol-water)	5.12
Henry's Law Constant	2.45E-08 atm-m ³ /mole
Boiling Point	309.5 °C
Melting Point	174 °C



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Specifications	Limits
Storage Temperature	0-6°C
Flash Point	11 °C
Merck	7109
Stability	Stable. Incompatible with strong oxidizing agents.

Specifications	Limits
Melting Point	165-180 °C
Vapor Density	9.2
Vapor Pressure	40 mm Hg (211.2 °C)
Density	1.978 g/mL at 25 °C
Boiling Point	310 °C



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