

Drometrizole

Other names:	Phenol, 2-(2H-benzotriazol-2-yl)-4-methyl- p-Cresol, 2-(2H-benzotriazol-2-yl)- Benazol P Tin P Tinuvin P UV Absorber-1 2-(2-Hydroxy-5-methylphenyl)benzotriazole 2-(2'-Hydroxy-5'-methylphenyl)benzotriazole 2-(2-Benzotriazolyl)-p-cresol 2-Benzotriazolyl-4-methylphenol 2-(2-Hydroxy-5-methylphenyl)-2H-benzotriazole Porex P 2-(2H-Benzotriazol-2-yl)-p-cresol 2-(2H-Benzotriazol-2-yl)-4-methylphenol Lowilite 55 Topanex 100BT Uvazol P NSC 91885
Inchi:	InChI=1S/C13H11N3O/c1-9-6-7-13(17)12(8-9)16-14-10-4-2-3-5-11(10)15-16/h2-8,17H,1
InchiKey:	MCPKSFINULVDNX-UHFFFAOYSA-N
Formula:	C13H11N3O
SMILES:	<chem>Cc1ccc(O)c(-n2nc3ccccc3n2)c1</chem>
Mol. weight [g/mol]:	225.25
CAS:	2440-22-4

Physical Properties

Property code	Value	Unit	Source
chs	-6744.00 ± 4.40	kJ/mol	NIST Webbook
chs	-6744.00 ± 4.40	kJ/mol	NIST Webbook
hfs	56.30 ± 4.50	kJ/mol	NIST Webbook
hfs	56.30 ± 4.50	kJ/mol	NIST Webbook
log10ws	-4.48		Crippen Method
logp	2.435		Crippen Method
mcvol	167.160	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	125.20	kJ/mol	313.00	NIST Webbook
hvapt	70.60	kJ/mol	419.50	NIST Webbook
hvapt	79.10	kJ/mol	423.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2440224&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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