

Pyrimidine, 2,4,6-trichloro-

Other names: 2,4,6-Trichloropyrimidine
Inchi: InChI=1S/C4HCl3N2/c5-2-1-3(6)9-4(7)8-2/h1H
InchiKey: DPVIABCMTHHTGB-UHFFFAOYSA-N
Formula: C4HCl3N2
SMILES: Clc1cc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 183.42
CAS: 3764-01-0

Physical Properties

Property code	Value	Unit	Source
hvap	55.60 ± 0.60	kJ/mol	NIST Webbook
log10ws	-3.06		Crippen Method
logp	2.437		Crippen Method
mcvol	100.140	ml/mol	McGowan Method
tb	485.70	K	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3764010&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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