

2,6-Dichloropyrazine

Other names: Pyrazine, 2,6-dichloro-
Inchi: InChI=1S/C4H2Cl2N2/c5-3-1-7-2-4(6)8-3/h1-2H
InchiKey: LSEAAPGIZCDEEH-UHFFFAOYSA-N
Formula: C4H2Cl2N2
SMILES: Clc1cncc(Cl)n1
Mol. weight [g/mol]: 148.98
CAS: 4774-14-5

Physical Properties

Property code	Value	Unit	Source
hsub	69.90 ± 2.00	kJ/mol	NIST Webbook
log10ws	-2.37		Crippen Method
logp	1.783		Crippen Method
mcvol	87.900	ml/mol	McGowan Method
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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=C4774145&Units=SI>

Legend

hsub: Enthalpy of sublimation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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