PYRAZINE, 2,6-DICHLORO-

Other names: 2,6-dichloropyrazine
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

Physical Properties

Property code	Value	Unit	Source
hsub	69.90 ± 2.00	kJ/mol	NIST Webbook
hvap	47.63	kJ/mol	Cheméo Relay (1.0)
logp	1.783		Crippen Method
mcvol	87.900	ml/mol	McGowan Method
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook
tb	453.59	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Thermochemical study of chloropyrazines and chloroquinoxalines: https://www.doi.org/10.1016/j.jct.2004.01.005

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4774145&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature