2,3-DICHLOROQUINOXALINE

Inchi: InChI=1S/C8H4Cl2N2/c9-7-8(10)12-6-4-2-1-3-5(6)11-7/h1-4H
InchiKey: SPSSDDOTEZKOOV-UHFFFAOYSA-N
Formula: C8H4Cl2N2
SMILES: Clc1nc2ccccc2nc1Cl
Mol. weight [g/mol]: 199.04

Physical Properties

Property code	Value	Unit	Source
hf	202.63	kJ/mol	Cheméo Relay (1.0)
hsub	91.80 ± 1.10	kJ/mol	NIST Webbook
hsub	93.10 ± 0.90	kJ/mol	NIST Webbook
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)
logp	2.937		Crippen Method
mcvol	124.800	ml/mol	McGowan Method
tb	549.40	K	Cheméo Relay (1.0)
tf	407.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.36	kJ/mol	424.40	NIST Webbook
hsubt	92.40 ± 0.40	kJ/mol	321.00	NIST Webbook

Sources

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=C2213630&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

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point