

Chloropyrazine

Other names:	2-Chloropyrazine Pyrazine, chloro-
Inchi:	InChI=1S/C4H3ClN2/c5-4-3-6-1-2-7-4/h1-3H
InchiKey:	GELVZYOEQVJIRR-UHFFFAOYSA-N
Formula:	C4H3ClN2
SMILES:	Clc1cnccn1
Mol. weight [g/mol]:	114.53
CAS:	14508-49-7

Physical Properties

Property code	Value	Unit	Source
hvap	45.10 ± 1.50	kJ/mol	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.130		Crippen Method
mcvol	75.660	ml/mol	McGowan Method
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	861.00		NIST Webbook
ripol	1351.00		NIST Webbook
tb	426.70	K	NIST Webbook

Sources

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=C14508497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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