

Pyrazine, 2,3-dichloro-

Other names:	2,3-Dichloropyrazine
Inchi:	InChI=1S/C4H2Cl2N2/c5-3-4(6)8-2-1-7-3/h1-2H
InchiKey:	MLCNOCRGSBCAGH-UHFFFAOYSA-N
Formula:	C4H2Cl2N2
SMILES:	Clc1nccnc1Cl
Mol. weight [g/mol]:	148.98
CAS:	4858-85-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.783		Crippen Method
mcvol	87.900	ml/mol	McGowan Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1581.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4858859&Units=SI

Legend

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

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