

Quinoxaline, 5-methyl-

Other names:	5-Methylquinoxaline
Inchi:	InChI=1S/C9H8N2/c1-7-3-2-4-8-9(7)11-6-5-10-8/h2-6H,1H3
InchiKey:	CQLOYHZZZCWHSG-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	Cc1cccc2ncnc12
Mol. weight [g/mol]:	144.17
CAS:	13708-12-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	1.938		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
ripol	1332.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1992.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	2.00	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=C13708128&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
tbrp:	Boiling point at reduced pressure

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