5,6,7,8-Tetrahydroquinoxaline

Other names: Quinoxaline, 5,6,7,8-tetrahydro-
Inchi: InChI=1S/C8H10N2/c1-2-4-8-7(3-1)9-5-6-10-8/h5-6H,1-4H2
InchiKey: XCZPDOCRSYZOBI-UHFFFAOYSA-N
Formula: C8H10N2
SMILES: c1cnc2c(n1)CCCC2
Mol. weight [g/mol]: 134.18
CAS: 34413-35-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	1.355		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
rinpol	1173.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1173.00		NIST Webbook
ripol	1717.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	0.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C34413359&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