

2(1H)-Quinoxalinone, 3-methyl-

Other names:	2-Hydroxy-3-methylquinoxaline 3-Methyl-2-quinoxalalone 2-Quinoxalinol, 3-methyl- 3-Methyl-2-quinoxalinol 3-Hydroxy-2-methylquinoxaline USAF el-7 3-Methyl-2(1H)-quinoxalinone 3-methylquinoxalin-2-ol 2-Methyl-3-hydroxyquinoxaline
Inchi:	InChI=1S/C9H8N2O/c1-6-9(12)11-8-5-3-2-4-7(8)10-6/h2-5H,1H3,(H,11,12)
InchiKey:	BMIMNRPAEPIYDN-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	Cc1nc2cccc2[nH]c1=O
Mol. weight [g/mol]:	160.17
CAS:	14003-34-0

Physical Properties

Property code	Value	Unit	Source
hsub	119.70 ± 2.80	kJ/mol	NIST Webbook
hsub	123.00 ± 4.40	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	0.750		Crippen Method
mcvol	120.280	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.40	kJ/mol	522.90	NIST Webbook
hsupt	117.20 ± 0.40	kJ/mol	383.00	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=C14003340&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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