2(1H)-Quinoxalinone

Other names:	Quinoxalin-2-one
	2-Hydroxyquinoxaline
	2-Quinoxalinol
	2-Quinoxalinone
	3-Quinoxalinone
	1,2-Dihydroquinoxalin-2-one
	2-Quinoxalone
	Quinoxalinone
	quinoxalin-2(1H)-one
Inchi:	InChI=1S/C8H6N2O/c11-8-5-9-6-3-1-2-4-7(6)10-8/h1-5H,(H,10,11)
InchiKey:	FFRYUAVNPBUEIC-UHFFFAOYSA-N
Formula:	C8H6N2O
SMILES:	O=c1cnc2ccccc2[nH]1
Mol. weight [g/mol]:	146.15
CAS:	1196-57-2

Physical Properties

Property code	Value	Unit	Source
hsub	118.50 ± 3.10	kJ/mol	NIST Webbook
hsub	125.80 ± 4.00	kJ/mol	NIST Webbook
log10ws	-1.68		Crippen Method
logp	0.441		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.50	kJ/mol	542.50	NIST Webbook
hsubt	116.10 ± 0.60	kJ/mol	391.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1196572&Units=SI
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

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