

8-Hydroxyquinaldine

Other names:	2-Methyl-8-hydroxyquinoline 2-Methyl-8-quinolinol 2-Methyloxine 8-Hydroxy-2-methylquinoline 8-Hydroxyquinaldine Hydroxyquinaldine 8-Hydroxyqinaldine 2-methylquinolin-8-ol
Inchi:	InChI=1S/C10H9NO/c1-7-5-6-8-3-2-4-9(12)10(8)11-7/h2-6,12H,1H3
InchiKey:	NBYLBWHHTUWMER-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	Cc1ccc2cccc(O)c2n1
Mol. weight [g/mol]:	159.19

Physical Properties

Property code	Value	Unit	Source
af	0.5732		Cheméo Relay (1.0)
chs	-5091.50 ± 1.60	kJ/mol	NIST Webbook
hf	-39.40 ± 2.20	kJ/mol	NIST Webbook
hfs	-129.80 ± 2.10	kJ/mol	NIST Webbook
hsub	90.40 ± 0.70	kJ/mol	NIST Webbook
hvap	79.63	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-1.61		Cheméo Relay (1.0)
logp	2.249		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
pc	5456.94	kPa	Cheméo Relay (1.0, beta)
tb	540.20	K	NIST Webbook
tc	847.21	K	Cheméo Relay (1.0)
tf	336.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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hsubt	90.40 ± 0.70	kJ/mol	301.50	NIST Webbook
hsubt	87.90	kJ/mol	320.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C826813&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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