

4-Quinolinol, 2-methyl-

Other names:	2-Methyl-4-quinolinol 2-Methyl-quinolin-4-ol 4-Hydroxy-2-methylquinoline 4-Hydroxyquinaldine
Inchi:	InChI=1S/C10H9NO/c1-7-6-10(12)8-4-2-3-5-9(8)11-7/h2-6H,1H3,(H,11,12)
InchiKey:	NWINIEGDLHHNLH-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	<chem>Cc1cc(O)c2ccccc2n1</chem>
Mol. weight [g/mol]:	159.18
CAS:	607-67-0

Physical Properties

Property code	Value	Unit	Source
chs	-5059.00 ± 2.40	kJ/mol	NIST Webbook
hf	-23.30 ± 2.90	kJ/mol	NIST Webbook
hfs	-162.30 ± 2.40	kJ/mol	NIST Webbook
hsub	139.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.20		Aqueous Solubility Prediction Method
logp	2.249		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
tf	507.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C607670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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