2-METHYL-4-QUINOLINOL

Other names:	2-Methyl-quinolin-4-ol
	4-Hydroxy-2-methylquinoline
	4-Hydroxyquinaldine
	4-Quinolinol, 2-methyl-
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:	Cc1cc(O)c2ccccc2n1
Mol. weight [g/mol]:	159.19

Physical Properties

Property code	Value	Unit	Source
af	0.5607		Cheméo Relay (1.0)
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
hvap	84.36	kJ/mol	Cheméo Relay (1.0)
ie	7.97	eV	Cheméo Relay (1.0)
log10ws	-1.20		Aqueous Solubility Prediction Method
logp	2.249		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
pc	5443.82	kPa	Cheméo Relay (1.0, beta)
tb	555.29	K	Cheméo Relay (1.0)
tc	848.69	K	Cheméo Relay (1.0)
tf	507.65	K	Aqueous Solubility Prediction Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C607670&Units=SI

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
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