

4-Methyl-2-hydroxyquinoline

Inchi: InChI=1S/C10H9NO/c1-7-6-10(12)11-9-5-3-2-4-8(7)9/h2-6H,1H3,(H,11,12)
InchiKey: APLVPBUBDFWWAD-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: Cc1cc(O)nc2ccccc12
Mol. weight [g/mol]: 159.18
CAS: 84909-43-3

Physical Properties

Property code	Value	Unit	Source
chs	-5032.20 ± 2.50	kJ/mol	NIST Webbook
hf	-61.00 ± 3.20	kJ/mol	NIST Webbook
hfs	-189.10 ± 2.80	kJ/mol	NIST Webbook
hsub	128.10 ± 1.60	kJ/mol	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.249		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

Sources

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=C84909433&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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