4-Quinolinol

Other names:	4-Hydroxyquinoline
	Kynurine
	quinolin-4-ol
Inchi:	InChI=1S/C9H7NO/c11-9-5-6-10-8-4-2-1-3-7(8)9/h1-6H,(H,10,11)
InchiKey:	PMZDQRJGMBOQBF-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	Oc1ccnc2ccccc12
Mol. weight [g/mol]:	145.16
CAS:	611-36-9

Physical Properties

Property code	Value	Unit	Source
chs	-4427.70 ± 1.60	kJ/mol	NIST Webbook
hf	20.80 ± 2.30	kJ/mol	NIST Webbook
hfs	-114.30 ± 2.00	kJ/mol	NIST Webbook
hsub	135.10 ± 1.10	kJ/mol	NIST Webbook
hsub	135.10 ± 1.10	kJ/mol	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-2.59		Crippen Method
logp	1.940		Crippen Method
mcvol	110.300	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	128.80 ± 1.10	kJ/mol	424.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611369&Units=SI

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
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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