

2,4-Quinolinediol

Other names:	2,4-Dihydroxyquinoline 2,4-Quinolinediol (mainly keto form) quinoline-2,4-diol
Inchi:	InChI=1S/C9H7NO2/c11-8-5-9(12)10-7-4-2-1-3-6(7)8/h1-5H,(H2,10,11,12)
InchiKey:	HDHQZCHIXUUSMK-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	O=c1cc(O)c2ccccc2[nH]1
Mol. weight [g/mol]:	161.16
CAS:	86-95-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	0.752		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
tf	626.00 ± 4.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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