

1H-Indol-5-ol

Other names:	Indol-5-ol 5-Hydroxy-1H-indole 5-Hydroxyindole Hydroxy-5 indole
Inchi:	InChI=1S/C8H7NO/c10-7-1-2-8-6(5-7)3-4-9-8/h1-5,9-10H
InchiKey:	LMIQERWZRIFWNZ-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	Oc1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	133.15
CAS:	1953-54-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.392		Crippen Method
mcvol	100.510	ml/mol	McGowan Method
rinpol	1660.00		NIST Webbook
tf	380.90 ± 1.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1953544&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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