

2-Isopropylimidazole

Other names:	1H-Imidazole, 2-(1-methylethyl)- 2-(1-methylethyl)-1H-imidazole 2-isopropyl-1H-imidazole
Inchi:	InChI=1S/C6H10N2/c1-5(2)6-7-3-4-8-6/h3-5H,1-2H3,(H,7,8)
InchiKey:	FUOZJYASZOSONT-UHFFFAOYSA-N
Formula:	C6H10N2
SMILES:	CC(C)c1ncc[nH]1
Mol. weight [g/mol]:	110.16
CAS:	36947-68-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.051		Crippen Method
mcvol	95.900	ml/mol	McGowan Method

Sources

Solubility of 2-isopropylimidazole in nine pure organic solvents and liquid mixtures of Methanol + ethyl acetate from T = (278.15 to 313.15) K: Experimental measurement and thermodynamic modelling:
Crippen Method:

<https://www.doi.org/10.1016/j.jct.2016.12.028>
<http://link.springer.com/article/10.1007/BF02311772>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C36947689&Units=SI>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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

Latest version available from:

<https://www.chemeo.com/cid/92-314-1/2-Isopropylimidazole.pdf>

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