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

Physical Properties

Property code	Value	Unit	Source
hf	26.99	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
logp	1.051		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
tb	514.46	K	Cheméo Relay (1.0)
tf	353.73	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36947689&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility of 2-isopropylimidazole in nine pure organic solvents and liquid mixture of (methanol + ethyl acetate) from T = (278.15 to 313.15) K: Experimental measurement and thermodynamic modelling:	https://www.doi.org/10.1016/j.jct.2016.12.028

Legend

hf:	Enthalpy of formation at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point