2-PROPYLBENZIMIDAZOLE

Other names:	1H-benzimidazole, 2-propyl-
	2-propyl-1H-benzimidazole
	Benzimidazole, 2-propyl-
Inchi:	InChI=1S/C10H12N2/c1-2-5-10-11-8-6-3-4-7-9(8)12-10/h3-4,6-7H,2,5H2,1H3,(H,11,12)
InchiKey:	FBLJZPQLNMVEMR-UHFFFAOYSA-N
Formula:	C10H12N2
SMILES:	CCCc1nc2ccccc2[nH]1
Mol. weight [g/mol]:	160.22

Physical Properties

Property code	Value	Unit	Source
hfus	1.50	kJ/mol	Experimental thermochemical study of two 2-alkylbenzimidazole isomers (alkyl=propyl and isopropyl)
hsub	109.40 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.55		Cheméo Relay (1.0)
logp	2.033		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
tf	416.00	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental thermochemical study of two 2-alkylbenzimidazole isomers (alkyl=propyl and isopropyl):	https://www.doi.org/10.1016/j.jct.2004.03.005
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5465292&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point