

1H-Imidazole, 1-(phenylmethyl)-

Other names:	Imidazole, 1-benzyl- N-Benzylimidazole 1-Benzylimidazole BI 1-Benzyl-1H-imidazole
Inchi:	InChI=1S/C10H10N2/c1-2-4-10(5-3-1)8-12-7-6-11-9-12/h1-7,9H,8H2
InchiKey:	KKKDZZRICRFGSD-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	c1ccc(Cn2ccnc2)cc1
Mol. weight [g/mol]:	158.20
CAS:	4238-71-5

Physical Properties

Property code	Value	Unit	Source
hsub	102.10 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.80		Crippen Method
logp	1.931		Crippen Method
mvol	128.500	ml/mol	McGowan Method
tb	583.20	K	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4238715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
tb: Normal Boiling Point Temperature

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