

1H-BENZIMIDAZOL-2-AMINE

Other names:	Benzimidazole, 2-amino- 2-Aminobenzimidazole 2-Iminobenzimidazoline USAF ek-4037 2-Benzimidazolamine 2-Amino-1H-benzimidazole benzimidazol-2-ylamine
Inchi:	InChI=1S/C7H7N3/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H,(H3,8,9,10)
InchiKey:	JWYUFVNJZUSCSM-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	<chem>Nc1nc2ccccc2[nH]1</chem>
Mol. weight [g/mol]:	133.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Cheméo Relay (1.0)
logp	0.663		Crippen Method
mcvol	100.510	ml/mol	McGowan Method
tf	505.10 ± 0.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C934327&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):	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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