1H-benzimidazole, 2-(methylthio)-

Other names:	Benzimidazole, 2-(methylthio)-
	S-Methyl-2-mercaptobenzimidazole
	2-(Methylmercapto)benzimidazole
	2-(Methylthio)benzimidazole
	2-Methylsulfanyl-1H-benzoimidazole
	2-(Methylsulfanyl)-1H-benzimidazole
	NSC 21699
Inchi:	InChI=1S/C8H8N2S/c1-11-8-9-6-4-2-3-5-7(6)10-8/h2-5H,1H3,(H,9,10)
InchiKey:	OCKJFOHZLXIAAT-UHFFFAOYSA-N
Formula:	C8H8N2S
SMILES:	CSc1nc2ccccc2[nH]1
Mol. weight [g/mol]:	164.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Cheméo Relay (1.0)
logp	1.803		Crippen Method
mcvol	120.970	ml/mol	McGowan Method
tf	433.86	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7152241&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):

Legend

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