methyl 2-benzimidazolecarbamate

Other names:	2-(methoxycarboxamido)benzimidazole
	Carbendazim
	methoxycarbonylaminobenzimidazole
	methyl 1H-benzimidazole-2-carbamate
Inchi:	InChI=1S/C9H9N3O2/c1-14-9(13)12-8-10-6-4-2-3-5-7(6)11-8/h2-5H,1H3,(H2,10,11,12,13
InchiKey:	TWFZGCMQGLPBSX-UHFFFAOYSA-N
Formula:	C9H9N3O2
SMILES:	COC(=O)Nc1nc2ccccc2[nH]1
Mol. weight [g/mol]:	191.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Cheméo Relay (1.0)
logp	1.259		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
tf	516.77	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):	
Solubility modelling, solvent effect and preferential solvation of carbendazim in aqueous co-solvent mixtures of dimethylformamide, methanol, ethanol and n-propanol:	https://www.doi.org/10.1016/j.jct.2018.08.001
Measurement and correlation of solubility of carbendazim in lower alcohols:	https://www.doi.org/10.1016/j.tca.2017.12.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point