

1H-Imidazole-1-carboxylic acid, 1,1-dimethylethyl ester

Other names:	1H-Imidazole-1-carboxylic acid, 1,1-dimethylethyl ester tert-butyl 1H-imidazole-1-carboxylate
Inchi:	InChI=1S/C8H12N2O2/c1-8(2,3)12-7(11)10-5-4-9-6-10/h4-6H,1-3H3
InchiKey:	MTBKGWHHOBHJMHJ-UHFFFAOYSA-N
Formula:	C8H12N2O2
SMILES:	CC(C)(C)OC(=O)n1ccnc1
Mol. weight [g/mol]:	168.20

Physical Properties

Property code	Value	Unit	Source
ie	9.54	eV	Cheméo Relay (1.0)
logp	1.666		Crippen Method
mcvol	131.520	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49761822&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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