

N-tert-Butoxycarbonylimidazole

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:	MTBKGWHHOBJMhj-UHFFFAOYSA-N
Formula:	C8H12N2O2
SMILES:	CC(C)(C)OC(=O)n1ccnc1
Mol. weight [g/mol]:	168.19
CAS:	49761-82-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	1.666		Crippen Method
mcvol	131.520	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49761822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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