

Dimethyl 4,5-imidazole-dicarboxylate

Other names:	Dimethyl imidazole-4,5-dicarboxylate Imidazole-4,5-dicarboxylic acid, dimethyl ester 1H-Imidazole-4,5-dicarboxylic acid, dimethyl ester
Inchi:	InChI=1S/C7H8N2O4/c1-12-6(10)4-5(7(11)13-2)9-3-8-4/h3H,1-2H3,(H,8,9)
InchiKey:	CUIWFAXEALIQJS-UHFFFAOYSA-N
Formula:	C7H8N2O4
SMILES:	COC(=O)c1nc[nH]c1C(=O)OC
Mol. weight [g/mol]:	184.15
CAS:	3304-70-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	-0.499		Crippen Method
mcvol	124.870	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3304709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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