

Ethyl 4-nitro-1h-imidazole-5-carboxylate

Inchi:	InChI=1S/C6H7N3O4/c1-2-13-6(10)4-5(9(11)12)8-3-7-4/h3H,2H2,1H3,(H,7,8)
InchiKey:	JFHZQABGMJXACV-UHFFFAOYSA-N
Formula:	C6H7N3O4
SMILES:	CCOC(=O)c1[nH]cnc1[N+](=O)[O-]
Mol. weight [g/mol]:	185.14
CAS:	74478-95-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	0.013		Crippen Method
mcvol	120.760	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74478958&Units=SI

Legend

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

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