

Acetic acid, 5-nitroimidazole-4-carboxamido-, ethyl ester

Inchi:	InChI=1S/C8H10N4O5/c1-2-17-5(13)3-9-8(14)6-7(12(15)16)11-4-10-6/h4H,2-3H2,1H3,(H
InchiKey:	FGPGXMNSQXMECL-UHFFFAOYSA-N
Formula:	C8H10N4O5
SMILES:	CCOC(=O)CNC(=O)c1nc[nH]c1[N+](=O)[O-]
Mol. weight [g/mol]:	242.19
CAS:	197912-16-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	-0.871		Crippen Method
mcvol	160.490	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C197912166&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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