

Imidazole-4-carboxamide, n-ethyl-5-nitro

Inchi:	InChI=1S/C6H8N4O3/c1-2-7-6(11)4-5(10(12)13)9-3-8-4/h3H,2H2,1H3,(H,7,11)(H,8,9)
InchiKey:	XZTGILDRMSNFQF-UHFFFAOYSA-N
Formula:	C6H8N4O3
SMILES:	CCNC(=O)c1[nH]cnc1[N+](=O)[O-]
Mol. weight [g/mol]:	184.15
CAS:	7509-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.87		Crippen Method
logp	-0.414		Crippen Method
mcvol	124.870	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=C7509968&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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