

5-Nitrofuran-2-carboxylic acid

Other names:	5-Nitro-2-furoic acid 2-Furancarboxylic acid, 5-nitro- 2-Furoic acid, 5-nitro- 5-Nitrofurancarboxylic acid Nitrofurate 5-Nitrofuroic acid 5-Nitropyromucic acid
Inchi:	InChI=1S/C5H3NO5/c7-5(8)3-1-2-4(11-3)6(9)10/h1-2H,(H,7,8)
InchiKey:	IODMEDPPCXSFLD-UHFFFAOYSA-N
Formula:	C5H3NO5
SMILES:	O=C(O)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]:	157.08
CAS:	645-12-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	0.886		Crippen Method
mcvol	92.580	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=C645125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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