

5-Nitrothiophene-2-carbonitrile

Inchi:	InChI=1S/C5H2N2O2S/c6-3-4-1-2-5(10-4)7(8)9/h1-2H
InchiKey:	FLYONFCGDKAMIH-UHFFFAOYSA-N
Formula:	C5H2N2O2S
SMILES:	N#Cc1ccc([N+](=O)[O-])s1
Mol. weight [g/mol]:	154.15
CAS:	16689-02-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	1.528		Crippen Method
mcvol	97.000	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C16689024&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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