

3-Aminothiophene-2-carboxamide

Inchi:	InChI=1S/C5H6N2OS/c6-3-1-2-9-4(3)5(7)8/h1-2H,6H2,(H2,7,8)
InchiKey:	BKDZTJNNXCNSCK-UHFFFAOYSA-N
Formula:	C5H6N2OS
SMILES:	NC(=O)c1sccc1N
Mol. weight [g/mol]:	142.18
CAS:	147123-47-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	0.429		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C147123475&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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