

Benzo(b)thiophene-2-carboxamide

Inchi:	InChI=1S/C9H7NOS/c10-9(11)8-5-6-3-1-2-4-7(6)12-8/h1-5H,(H2,10,11)
InchiKey:	GYSCBCSGKXNZRH-UHFFFAOYSA-N
Formula:	C9H7NOS
SMILES:	NC(=O)c1cc2ccccc2s1
Mol. weight [g/mol]:	177.22
CAS:	6314-42-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.000		Crippen Method
mcvol	126.650	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6314427&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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