Thianaphthene-3-acetonirile

Other names:	Benzo[b]thiophene-3-acetonitrile
	Acetonitrile, 2-(3-benzothieny)-
	1-Benzothien-3-ylacetonitrile
Inchi:	InChI=1S/C10H7NS/c11-6-5-8-7-12-10-4-2-1-3-9(8)10/h1-4,7H,5H2
InchiKey:	DEELHLMCCWZFFE-UHFFFAOYSA-N
Formula:	C10H7NS
SMILES:	N#CCc1csc2ccccc12
Mol. weight [g/mol]:	173.23
CAS:	3216-48-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	2.967		Crippen Method
mcvol	130.570	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=C3216486&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume