

Benzo[b]thiophene-3-ethylamine, alpha-methyl-

Inchi:	InChI=1S/C11H13NS/c1-8(12)6-9-7-13-11-5-3-2-4-10(9)11/h2-5,7-8H,6,12H2,1H3
InchiKey:	NJJBOBSLFFUELD-UHFFFAOYSA-N
Formula:	C11H13NS
SMILES:	CC(N)Cc1csc2ccccc12
Mol. weight [g/mol]:	191.29
CAS:	1201-27-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.791		Crippen Method
mcvol	153.260	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1201270&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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