

Ethyl 2-amino-4-methylthiophene-3-carboxylate

Inchi:	InChI=1S/C8H11NO2S/c1-3-11-8(10)6-5(2)4-12-7(6)9/h4H,3,9H2,1-2H3
InchiKey:	ILYCZKOBRLRJJSSW-UHFFFAOYSA-N
Formula:	C8H11NO2S
SMILES:	CCOC(=O)c1c(C)csc1N
Mol. weight [g/mol]:	185.24
CAS:	43088-42-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.815		Crippen Method
mcvol	137.890	ml/mol	McGowan Method

Sources

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=C43088422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/55-015-4/Ethyl-2-amino-4-methylthiophene-3-carboxylate.pdf>

Generated by Cheméo on 2024-05-03 09:03:40.806782927 +0000 UTC m=+17016269.727360243.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.