

Methyl benzo[b]thiophene-2-carboxylate

Inchi:	InChI=1S/C10H8O2S/c1-12-10(11)9-6-7-4-2-3-5-8(7)13-9/h2-6H,1H3
InchiKey:	KRRAZMUPVIGDCU-UHFFFAOYSA-N
Formula:	C10H8O2S
SMILES:	<chem>COC(=O)c1cc2ccccc2s1</chem>
Mol. weight [g/mol]:	192.23
CAS:	22913-24-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.688		Crippen Method
mcvol	136.630	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22913242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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