

Benzo[b]thiophene-2-carboxaldehyde, 7-methyl-

Inchi:	InChI=1S/C10H8OS/c1-7-3-2-4-8-5-9(6-11)12-10(7)8/h2-6H,1H3
InchiKey:	MLLVSGDRQOXPNS-UHFFFAOYSA-N
Formula:	C10H8OS
SMILES:	Cc1cccc2cc(C=O)sc12
Mol. weight [g/mol]:	176.24
CAS:	3751-76-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	3.022		Crippen Method
mcvol	130.760	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=C3751766&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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