

2-Furancarbothioic acid, S-methyl ester

Other names:	2-Furoic acid, thio-, S-methyl ester Methyl 2-thiofuroate Methylthiol furoate S-Methyl thiofuroate S-Methyl 2-furancarbothioate Methyl thiofuroate methyl thio-2-furoate
Inchi:	InChI=1S/C6H6O2S/c1-9-6(7)5-3-2-4-8-5/h2-4H,1H3
InchiKey:	ISKUAGFDTRLBHG-UHFFFAOYSA-N
Formula:	C6H6O2S
SMILES:	CSC(=O)c1ccco1
Mol. weight [g/mol]:	142.18
CAS:	13679-61-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	1.783		Crippen Method
mvol	99.730	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679613&Units=SI
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

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.cheméo.com/cid/98-609-8/2-Furancarbothioic-acid-S-methyl-ester.pdf>

Generated by Cheméo on 2024-04-20 14:53:27.005996588 +0000 UTC m=+15914055.926573904.

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