

3-formyl-2-methylthiophene

Other names:	2-Methylthiophene-3-carboxaldehyde 2-Methyl-3-formylthiophene Thiophen-3-carboxaldehyde, 2-methyl
Inchi:	InChI=1S/C6H6OS/c1-5-6(4-7)2-3-8-5/h2-4H,1H3
InchiKey:	NSYHYZOBGJOIMD-UHFFFAOYSA-N
Formula:	C6H6OS
SMILES:	Cc1sccc1C=O
Mol. weight [g/mol]:	126.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.869		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1089.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1091.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R69813&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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