

3-Methyl-2-thiophenecarboxaldehyde

Other names:	3-Methylthiophene-2-carboxaldehyde 3-Methylthiophene-2-aldehyde 2-Thiophenecarboxaldehyde, 3-methyl- 3-Methyl-2-thiophenecarbaldehyde 2-Formyl-3-methylthiophene 3-Methyl-2-carboxaldehyde-thiophene 3-Methyl-2-formylthiophene 3-Methyl-2-thiophencarboxaldehyde 3-Methylthiophen-2-carboxaldehyde Thiophene, 3-Methyl, 2-formyl 3-Methylthiophene-2-carbaldehyde 3-Methyl-2-thiophenecarboxyaldehyde
Inchi:	InChI=1S/C6H6OS/c1-5-2-3-8-6(5)4-7/h2-4H,1H3
InchiKey:	BSQKBHXYEKVKMN-UHFFFAOYSA-N
Formula:	C6H6OS
SMILES:	Cc1ccsc1C=O
Mol. weight [g/mol]:	126.18
CAS:	5834-16-2

Physical Properties

Property code	Value	Unit	Source
hvap	56.20 ± 1.20	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.869		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1104.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1092.00		NIST Webbook

rinpol	1105.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1089.00	NIST Webbook
ripol	1797.00	NIST Webbook
ripol	1765.00	NIST Webbook
ripol	1813.00	NIST Webbook
ripol	1814.00	NIST Webbook
ripol	1815.00	NIST Webbook
ripol	1761.00	NIST Webbook

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=C5834162&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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