

5-Methyl-2-thiophenecarboxaldehyde

Other names:	5-Methylthiophene-2-aldehyde 5-Methylthiophene-2-carboxaldehyde 2-Thiophenecarboxaldehyde, 5-methyl- 2-Formyl-5-methylthiophene 5-Methyl-2-formylthiophene 5-Methyl-2-thiophenecarboxaldehyde 5-Methyl-2-thiophenecarbaldehyde 5-Methyl-2-carboxaldehyde-thiophene Thiophen-2-carboxaldehyde, 5-methyl Thiophene, 2-Methyl, 5-formyl 5-methylthiophene-2-carbaldehyde
Inchi:	InChI=1S/C6H6OS/c1-5-2-3-6(4-7)8-5/h2-4H,1H3
InchiKey:	VAUMDUIUEPIGHM-UHFFFAOYSA-N
Formula:	C6H6OS
SMILES:	<chem>Cc1ccc(C=O)s1</chem>
Mol. weight [g/mol]:	126.18
CAS:	13679-70-4

Physical Properties

Property code	Value	Unit	Source
hvap	57.70 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.869		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1087.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1060.00		NIST Webbook

rinpol	1086.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1116.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1077.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1116.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1087.00	NIST Webbook
ripol	1797.00	NIST Webbook
ripol	1767.00	NIST Webbook
ripol	1759.00	NIST Webbook
ripol	1755.00	NIST Webbook
ripol	1744.00	NIST Webbook
ripol	1744.00	NIST Webbook
ripol	1783.00	NIST Webbook
ripol	1781.00	NIST Webbook
ripol	1780.00	NIST Webbook
ripol	1739.00	NIST Webbook
ripol	1797.00	NIST Webbook
ripol	1785.00	NIST Webbook
ripol	1767.00	NIST Webbook
ripol	1782.00	NIST Webbook
ripol	1765.00	NIST Webbook
ripol	1767.00	NIST Webbook
ripol	1735.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	3.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C13679704&Units=SI

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure

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