

2,5-Thiophenedicarboxaldehyde

Other names:	2,5-Diformylthiophene 2,5-Thiophenedial 2,5-Thiophenedicarbaldehyde Thiophene-2,5-dicarbaldehyde 2,5-Diformylthiophen
Inchi:	InChI=1S/C6H4O2S/c7-3-5-1-2-6(4-8)9-5/h1-4H
InchiKey:	OTMRXENQDSQACG-UHFFFAOYSA-N
Formula:	C6H4O2S
SMILES:	O=Cc1ccc(C=O)s1
Mol. weight [g/mol]:	140.16
CAS:	932-95-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	1.373		Crippen Method
mcvol	95.430	ml/mol	McGowan Method
rinpol	1220.00		NIST Webbook
ripol	1833.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932956&Units=SI

Legend

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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