

2,5-DIFORMYLTHIOPHENE

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

Physical Properties

Property code	Value	Unit	Source
hvap	71.09	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
logp	1.373		Crippen Method
mcvol	95.430	ml/mol	McGowan Method
rinpol	1220.00		NIST Webbook
ripol	1833.00		NIST Webbook
tb	526.27	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932956&Units=SI

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature

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