

Di-2-thienyl ketone

Other names:	Methanone, di-2-thienyl- 2-Thienyl ketone
Inchi:	InChI=1S/C9H6OS2/c10-9(7-3-1-5-11-7)8-4-2-6-12-8/h1-6H
InchiKey:	GUTQMBQKTSGBPQ-UHFFFAOYSA-N
Formula:	C9H6OS2
SMILES:	O=C(c1cccs1)c1cccs1
Mol. weight [g/mol]:	194.27
CAS:	704-38-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	3.041		Crippen Method
mcvol	133.020	ml/mol	McGowan Method

Sources

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=C704381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/51-196-8/Di-2-thienyl-ketone.pdf>

Generated by Cheméo on 2024-04-30 15:03:14.803993787 +0000 UTC m=+16778643.724571097.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.