

2-Thiopheneacetyl chloride

Other names:	Thiophene-2-acetyl chloride 2-Thienylacetyl chloride
Inchi:	InChI=1S/C6H5ClOS/c7-6(8)4-5-2-1-3-9-5/h1-3H,4H2
InchiKey:	AJYXPNIENRLELY-UHFFFAOYSA-N
Formula:	C6H5ClOS
SMILES:	O=C(Cl)Cc1cccs1
Mol. weight [g/mol]:	160.62
CAS:	39098-97-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	2.056		Crippen Method
mcvol	106.100	ml/mol	McGowan Method
rinpol	1162.00		NIST Webbook
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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=C39098970&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
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/44-112-8/2-Thiopheneacetyl-chloride.pdf>

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