

2-Thiophenecarbonyl chloride

Other names:	Thiophene-2-carbonyl chloride «alpha»-Thenoyl chloride 2-Thenoyl chloride 2-Thienylcarbonyl chloride
Inchi:	InChI=1S/C5H3ClOS/c6-5(7)4-2-1-3-8-4/h1-3H
InchiKey:	QIQITDHWZYEEPA-UHFFFAOYSA-N
Formula:	C5H3ClOS
SMILES:	O=C(Cl)c1cccs1
Mol. weight [g/mol]:	146.59
CAS:	5271-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	2.127		Crippen Method
mvol	92.010	ml/mol	McGowan Method
tb	480.20	K	NIST Webbook

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=C5271670&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
mvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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