

Thiophene, 2-(chloromethyl)-

Other names:	2-(Chloromethyl)-thiophene
Inchi:	InChI=1S/C5H5ClS/c6-4-5-2-1-3-7-5/h1-3H,4H2
InchiKey:	FUOHKPSBGLXIRL-UHFFFAOYSA-N
Formula:	C5H5ClS
SMILES:	ClCc1cccs1
Mol. weight [g/mol]:	132.61
CAS:	765-50-4

Physical Properties

Property code	Value	Unit	Source
ie	8.89 ± 0.05	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.487		Crippen Method
mcvol	90.440	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765504&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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