«gamma»-Chloro-2-butyrothienone

Other names:	1-Butanone, 4-chloro-1-(2-thienyl)-
	4-Chloro-1-(2-thienyl)butan-1-one
Inchi:	InChI=1S/C8H9ClOS/c9-5-1-3-7(10)8-4-2-6-11-8/h2,4,6H,1,3,5H2
InchiKey:	NPFQPHILVMHTKP-UHFFFAOYSA-N
Formula:	C8H9ClOS
SMILES:	O=C(CCCCl)c1cccs1
Mol. weight [g/mol]:	188.67
CAS:	43076-59-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.950		Crippen Method
mcvol	134.280	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=C43076591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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