1-BUTANONE, 4-CHLORO-1-(2-THIENYL)-

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]: 188.68

Physical Properties

Property code	Value	Unit	Source
hvap	70.27	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
logp	2.950		Crippen Method
mcvol	134.280	ml/mol	McGowan Method
tb	538.68	K	Cheméo Relay (1.0)
tf	292.70	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C43076591&Units=SI

Legend

hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point