2-(CHLORMETHYL)-TIOPHENE

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]: 132.62

Physical Properties

Property code	Value	Unit	Source
hf	25.53	kJ/mol	Cheméo Relay (1.0)
hvap	46.00	kJ/mol	Cheméo Relay (1.0)
ie	8.89 ± 0.05	eV	NIST Webbook
log10ws	-2.18		Cheméo Relay (1.0)
logp	2.487		Crippen Method
mcvol	90.440	ml/mol	McGowan Method
pc	4283.70	kPa	Cheméo Relay (1.0, beta)
tb	459.76	K	Cheméo Relay (1.0)
tc	680.21	K	Cheméo Relay (1.0)
tf	266.23	K	Cheméo Relay (1.0)
vc	0.312	m3/kmol	Cheméo Relay (1.0)

Sources

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=C765504&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume