2-(mercaptoethyl)tetrahydrothiophene

Inchi: InChI=1S/C6H12S2/c7-4-3-6-2-1-5-8-6/h6-7H,1-5H2
InchiKey: OLWFCZMLLCFXBT-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: SCCC1CCCS1
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	105.44	kJ/mol	Joback Method
hf	-22.95	kJ/mol	Joback Method
hfus	12.93	kJ/mol	Joback Method
hvap	41.76	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.202		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1117.00		NIST Webbook
tb	462.65	K	Joback Method
tc	702.26	K	Joback Method
tf	288.19	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.82	J/mol×K	462.65	Joback Method
cpg	244.69	J/mol×K	502.59	Joback Method
cpg	258.60	J/mol×K	542.52	Joback Method
cpg	271.60	J/mol×K	582.46	Joback Method
cpg	283.74	J/mol×K	622.39	Joback Method
cpg	295.05	J/mol×K	662.33	Joback Method
cpg	305.58	J/mol×K	702.26	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume