2-Mercapto-3,4-dimethyl-2,3-dihydrothiophene

Inchi: InChI=1S/C6H10S2/c1-4-3-8-6(7)5(4)2/h3,5-7H,1-2H3
InchiKey: VNWDIRWAEAIXKU-UHFFFAOYSA-N
Formula: C6H10S2
SMILES: CC1=CSC(S)C1C
Mol. weight [g/mol]: 146.27

Physical Properties

Property code	Value	Unit	Source
gf	118.06	kJ/mol	Joback Method
hf	3.02	kJ/mol	Joback Method
hfus	14.83	kJ/mol	Joback Method
hvap	42.40	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.529		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1149.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1149.00		NIST Webbook
tb	462.12	K	Joback Method
tc	705.66	K	Joback Method
tf	297.23	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.07	J/mol×K	462.12	Joback Method
cpg	229.33	J/mol×K	502.71	Joback Method
cpg	241.81	J/mol×K	543.30	Joback Method
cpg	253.53	J/mol×K	583.89	Joback Method
cpg	264.52	J/mol×K	624.48	Joback Method
cpg	274.80	J/mol×K	665.07	Joback Method
cpg	284.41	J/mol×K	705.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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