2-methyl-2-tetrahydrothiophenethiol

Inchi: InChI=1S/C5H10S2/c1-5(6)3-2-4-7-5/h6H,2-4H2,1H3
InchiKey: SVPXVYCUWKYTRA-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: CC1(S)CCCS1
Mol. weight [g/mol]: 134.26

Physical Properties

Property code	Value	Unit	Source
gf	91.53	kJ/mol	Joback Method
hf	12.93	kJ/mol	Joback Method
hfus	4.04	kJ/mol	Joback Method
hvap	38.38	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.159		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	440.01	K	Joback Method
tc	695.57	K	Joback Method
tf	300.82	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.31	J/mol×K	440.01	Joback Method
cpg	204.11	J/mol×K	482.60	Joback Method
cpg	216.56	J/mol×K	525.20	Joback Method
cpg	227.86	J/mol×K	567.79	Joback Method
cpg	238.19	J/mol×K	610.38	Joback Method
cpg	247.73	J/mol×K	652.97	Joback Method

cpg	256.68	J/mol×K	695.57	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=R169229&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume