3-Mercapto-2-methylpentanal, # 2

Inchi: InChI=1S/C6H12OS/c1-3-6(8)5(2)4-7/h4-6,8H,3H2,1-2H3
InchiKey: FSAGSGCELJTQFN-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CCC(S)C(C)C=O
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-75.37	kJ/mol	Joback Method
hf	-224.83	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	41.63	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.530		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	995.00		NIST Webbook
tb	447.32	K	Joback Method
tc	652.02	K	Joback Method
tf	205.84	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.84	J/mol×K	447.32	Joback Method
cpg	234.98	J/mol×K	481.44	Joback Method
cpg	245.59	J/mol×K	515.55	Joback Method
cpg	255.66	J/mol×K	549.67	Joback Method
cpg	265.22	J/mol×K	583.79	Joback Method
cpg	274.28	J/mol×K	617.90	Joback Method
cpg	282.85	J/mol×K	652.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R602994&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

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