3-mercaptobutyl-acetate

Inchi: InChI=1S/C6H12O2S/c1-5(9)3-4-8-6(2)7/h5,9H,3-4H2,1-2H3
InchiKey: GMXSGLCDVHHWIB-UHFFFAOYSA-N
Formula: C6H12O2S
SMILES: CC(=O)OCCC(C)S
Mol. weight [g/mol]: 148.22

Physical Properties

Property code	Value	Unit	Source
gf	-207.33	kJ/mol	Joback Method
hf	-378.77	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	44.45	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.258		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1559.00		NIST Webbook
tb	475.39	K	Joback Method
tc	679.41	K	Joback Method
tf	251.00	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.02	J/mol×K	475.39	Joback Method
cpg	254.95	J/mol×K	509.39	Joback Method
cpg	265.43	J/mol×K	543.40	Joback Method
cpg	275.45	J/mol×K	577.40	Joback Method
cpg	285.02	J/mol×K	611.41	Joback Method
cpg	294.14	J/mol×K	645.41	Joback Method

cpg	302.80	J/mol×K	679.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R291811&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume