1-Mercaptobutyl-3-acetate

Inchi: InChI=1S/C6H12O2S/c1-5(3-4-9)8-6(2)7/h5,9H,3-4H2,1-2H3
InchiKey: PPGZGGPLMMKFKW-UHFFFAOYSA-N
Formula: C6H12O2S
SMILES: CC(=O)OC(C)CCS
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	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1539.00		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

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=R291722&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