3-Methyl-3-sulfanylbutyl Butanoate

Inchi: InChI=1S/C9H18O2S/c1-4-5-8(10)11-7-6-9(2,3)12/h12H,4-7H2,1-3H3
InchiKey: GPJBVDXMTSFSPB-UHFFFAOYSA-N
Formula: C9H18O2S
SMILES: CCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 190.30

Physical Properties

Property code	Value	Unit	Source
gf	-176.79	kJ/mol	Joback Method
hf	-444.16	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.428		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	1266.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1725.00		NIST Webbook
tb	541.24	K	Joback Method
tc	744.68	K	Joback Method
tf	302.23	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.36	J/mol×K	541.24	Joback Method
cpg	392.98	J/mol×K	575.15	Joback Method
cpg	406.82	J/mol×K	609.05	Joback Method
cpg	419.89	J/mol×K	642.96	Joback Method
cpg	432.24	J/mol×K	676.87	Joback Method
cpg	443.87	J/mol×K	710.78	Joback Method
cpg	454.82	J/mol×K	744.68	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=R519550&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