sec-butyl 3-(methylthio)propanoate

Inchi: InChI=1S/C8H16O2S/c1-4-7(2)10-8(9)5-6-11-3/h7H,4-6H2,1-3H3
InchiKey: XHZHFZXKXPLJMV-UHFFFAOYSA-N
Formula: C8H16O2S
SMILES: CCC(C)OC(=O)CCSC
Mol. weight [g/mol]: 176.28

Physical Properties

Property code	Value	Unit	Source
gf	-186.76	kJ/mol	Joback Method
hf	-416.66	kJ/mol	Joback Method
hfus	19.87	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.081		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
ripol	1647.00		NIST Webbook
tb	527.07	K	Joback Method
tc	725.43	K	Joback Method
tf	271.48	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.94	J/mol×K	527.07	Joback Method
cpg	345.16	J/mol×K	560.13	Joback Method
cpg	357.82	J/mol×K	593.19	Joback Method
cpg	369.91	J/mol×K	626.25	Joback Method
cpg	381.43	J/mol×K	659.31	Joback Method
cpg	392.38	J/mol×K	692.37	Joback Method
cpg	402.77	J/mol×K	725.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327381&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume