butyl 3-(methylthio)propanoate

Inchi: InChI=1S/C8H16O2S/c1-3-4-6-10-8(9)5-7-11-2/h3-7H2,1-2H3
InchiKey: AOUVGXHIHWHVEM-UHFFFAOYSA-N
Formula: C8H16O2S
SMILES: CCCCOC(=O)CCSC
Mol. weight [g/mol]: 176.28

Physical Properties

Property code	Value	Unit	Source
gf	-184.32	kJ/mol	Joback Method
hf	-411.38	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.083		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
ripol	1748.00		NIST Webbook
tb	527.51	K	Joback Method
tc	721.73	K	Joback Method
tf	286.48	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.65	J/mol×K	527.51	Joback Method
cpg	344.52	J/mol×K	559.88	Joback Method
cpg	356.87	J/mol×K	592.25	Joback Method
cpg	368.68	J/mol×K	624.62	Joback Method
cpg	379.96	J/mol×K	656.99	Joback Method
cpg	390.70	J/mol×K	689.36	Joback Method
cpg	400.90	J/mol×K	721.73	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327183&Units=SI

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