Ethyl 4-(methylthio)butanoate

Other names: ethyl 4-(methylthio)butyrate
Inchi: InChI=1S/C7H14O2S/c1-3-9-7(8)5-4-6-10-2/h3-6H2,1-2H3
InchiKey: QNLREUZIHJHXRK-UHFFFAOYSA-N
Formula: C7H14O2S
SMILES: CCOC(=O)CCCSC
Mol. weight [g/mol]: 162.25
CAS: 22014-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-192.74	kJ/mol	Joback Method
hf	-390.74	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	47.15	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.693		Crippen Method
mcvol	133.280	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1652.00		NIST Webbook
tb	504.63	K	Joback Method
tc	701.40	K	Joback Method
tf	275.21	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.52	J/mol×K	504.63	Joback Method
cpg	299.37	J/mol×K	537.42	Joback Method
cpg	310.75	J/mol×K	570.22	Joback Method
cpg	321.65	J/mol×K	603.01	Joback Method

cpg	332.08	J/mol×K	635.81	Joback Method
cpg	342.03	J/mol×K	668.60	Joback Method
cpg	351.49	J/mol×K	701.40	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=C22014488&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