pentyl 3-(methylthio)propanoate

Inchi: InChI=1S/C9H18O2S/c1-3-4-5-7-11-9(10)6-8-12-2/h3-8H2,1-2H3
InchiKey: VSCXQPTWKZWPQB-UHFFFAOYSA-N
Formula: C9H18O2S
SMILES: CCCCCOC(=O)CCSC
Mol. weight [g/mol]: 190.30

Physical Properties

Property code	Value	Unit	Source
gf	-175.90	kJ/mol	Joback Method
hf	-432.02	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	51.60	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.473		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
ripol	1858.00		NIST Webbook
tb	550.39	K	Joback Method
tc	742.14	K	Joback Method
tf	297.75	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.69	J/mol×K	550.39	Joback Method
cpg	391.47	J/mol×K	582.35	Joback Method
cpg	404.66	J/mol×K	614.31	Joback Method
cpg	417.26	J/mol×K	646.27	Joback Method
cpg	429.28	J/mol×K	678.23	Joback Method
cpg	440.71	J/mol×K	710.19	Joback Method
cpg	451.55	J/mol×K	742.14	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=U122032&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