3-(Methylthio)propyl nonanoate

Inchi: InChI=1S/C13H26O2S/c1-3-4-5-6-7-8-10-13(14)15-11-9-12-16-2/h3-12H2,1-2H3
InchiKey: PPVJDHJFJZVMPX-UHFFFAOYSA-N
Formula: C13H26O2S
SMILES: CCCCCCCCC(=O)OCCCSC
Mol. weight [g/mol]: 246.41

Physical Properties

Property code	Value	Unit	Source
gf	-142.22	kJ/mol	Joback Method
hf	-514.58	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	60.50	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.033		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1819.00		NIST Webbook
tb	641.91	K	Joback Method
tc	825.75	K	Joback Method
tf	342.83	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.79	J/mol×K	641.91	Joback Method
cpg	595.17	J/mol×K	672.55	Joback Method
cpg	610.78	J/mol×K	703.19	Joback Method
cpg	625.64	J/mol×K	733.83	Joback Method
cpg	639.74	J/mol×K	764.47	Joback Method
cpg	653.10	J/mol×K	795.11	Joback Method
cpg	665.74	J/mol×K	825.75	Joback Method

Sources

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=U378255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume