3-(Methylthio)hexyl hexanoate

Inchi: InChI=1S/C13H26O2S/c1-4-6-7-9-13(14)15-11-10-12(16-3)8-5-2/h12H,4-11H2,1-3H3
InchiKey: YCHLQQVZMIQEAC-UHFFFAOYSA-N
Formula: C13H26O2S
SMILES: CCCCCC(=O)OCCC(CCC)SC
Mol. weight [g/mol]: 246.41
CAS: 136954-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-144.66	kJ/mol	Joback Method
hf	-519.86	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.032		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
ripol	2115.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2115.00		NIST Webbook
tb	641.47	K	Joback Method
tc	828.33	K	Joback Method
tf	327.83	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.22	J/mol×K	641.47	Joback Method
cpg	595.90	J/mol×K	672.61	Joback Method
cpg	611.79	J/mol×K	703.76	Joback Method
cpg	626.88	J/mol×K	734.90	Joback Method
cpg	641.19	J/mol×K	766.04	Joback Method
cpg	654.73	J/mol×K	797.19	Joback Method

cpg	667.51	J/mol×K	828.33	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=C136954240&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume