3-(hexanoylthio) hexyl hexanoate

Inchi: InChI=1S/C18H34O3S/c1-4-7-9-12-17(19)21-15-14-16(11-6-3)22-18(20)13-10-8-5-2/h16
InchiKey: HVKJBXIPCUJLMA-UHFFFAOYSA-N
Formula: C18H34O3S
SMILES: CCCCCC(=O)OCCC(CCC)SC(=O)CCCCC
Mol. weight [g/mol]: 330.53

Physical Properties

Property code	Value	Unit	Source
gf	-231.48	kJ/mol	Joback Method
hf	-735.64	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	77.99	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.509		Crippen Method
mcvol	289.840	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
ripol	2608.00		NIST Webbook
ripol	2608.00		NIST Webbook
tb	809.74	K	Joback Method
tc	1001.80	K	Joback Method
tf	434.11	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.45	J/mol×K	809.74	Joback Method
cpg	902.48	J/mol×K	841.75	Joback Method
cpg	918.46	J/mol×K	873.76	Joback Method
cpg	933.41	J/mol×K	905.77	Joback Method
cpg	947.35	J/mol×K	937.78	Joback Method
cpg	960.30	J/mol×K	969.79	Joback Method
cpg	972.28	J/mol×K	1001.80	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=R317641&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