3-(butanoylthio)hexyl butanoate

Inchi: InChI=1S/C14H26O3S/c1-4-7-12(18-14(16)9-6-3)10-11-17-13(15)8-5-2/h12H,4-11H2,1-3
InchiKey: IAAVYXKIYUAQRX-UHFFFAOYSA-N
Formula: C14H26O3S
SMILES: CCCC(=O)OCCC(CCC)SC(=O)CCC
Mol. weight [g/mol]: 274.42

Physical Properties

Property code	Value	Unit	Source
gf	-265.16	kJ/mol	Joback Method
hf	-653.08	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.948		Crippen Method
mcvol	233.480	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
ripol	2214.00		NIST Webbook
ripol	2214.00		NIST Webbook
tb	718.22	K	Joback Method
tc	910.73	K	Joback Method
tf	389.03	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.11	J/mol×K	718.22	Joback Method
cpg	671.89	J/mol×K	750.31	Joback Method
cpg	686.78	J/mol×K	782.39	Joback Method
cpg	700.80	J/mol×K	814.48	Joback Method
cpg	713.96	J/mol×K	846.56	Joback Method
cpg	726.26	J/mol×K	878.65	Joback Method
cpg	737.72	J/mol×K	910.73	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=R317636&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