3-(Methylthio)hexyl butanoate

Inchi: InChI=1S/C11H22O2S/c1-4-6-10(14-3)8-9-13-11(12)7-5-2/h10H,4-9H2,1-3H3
InchiKey: CPZRKTMCYSRJPH-UHFFFAOYSA-N
Formula: C11H22O2S
SMILES: CCCC(=O)OCCC(CCC)SC
Mol. weight [g/mol]: 218.36
CAS: 136954-23-9

Physical Properties

Property code	Value	Unit	Source
gf	-161.50	kJ/mol	Joback Method
hf	-478.58	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.252		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
ripol	1918.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	595.71	K	Joback Method
tc	786.50	K	Joback Method
tf	305.29	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.44	J/mol×K	595.71	Joback Method
cpg	491.03	J/mol×K	627.51	Joback Method
cpg	505.90	J/mol×K	659.31	Joback Method
cpg	520.05	J/mol×K	691.11	Joback Method
cpg	533.49	J/mol×K	722.90	Joback Method
cpg	546.24	J/mol×K	754.70	Joback Method

cpg	558.28	J/mol×K	786.50	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=C136954239&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