3-Methyl-3-sulfanylbutyl Hexanoate

Inchi: InChI=1S/C11H22O2S/c1-4-5-6-7-10(12)13-9-8-11(2,3)14/h14H,4-9H2,1-3H3
InchiKey: OBTUFRVSTPEASS-UHFFFAOYSA-N
Formula: C11H22O2S
SMILES: CCCCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 218.36

Physical Properties

Property code	Value	Unit	Source
gf	-159.95	kJ/mol	Joback Method
hf	-485.44	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.208		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1468.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1920.00		NIST Webbook
tb	587.00	K	Joback Method
tc	784.70	K	Joback Method
tf	324.77	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.94	J/mol×K	587.00	Joback Method
cpg	490.93	J/mol×K	619.95	Joback Method
cpg	506.06	J/mol×K	652.90	Joback Method
cpg	520.38	J/mol×K	685.85	Joback Method
cpg	533.90	J/mol×K	718.80	Joback Method
cpg	546.66	J/mol×K	751.75	Joback Method
cpg	558.69	J/mol×K	784.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519590&Units=SI
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

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