3-Methyl-3-sulfanylbutyl Hexadecanoate

Inchi: InChI=1S/C21H42O2S/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(22)23-19-18-21(2,3)2
InchiKey: KLURJANGYPXWHJ-UHFFFAOYSA-N
Formula: C21H42O2S
SMILES: CCCCCCCCCCCCCCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 358.62

Physical Properties

Property code	Value	Unit	Source
gf	-75.75	kJ/mol	Joback Method
hf	-691.84	kJ/mol	Joback Method
hfus	49.56	kJ/mol	Joback Method
hvap	76.94	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.109		Crippen Method
mcvol	330.540	ml/mol	McGowan Method
pc	1037.23	kPa	Joback Method
rinpol	2492.00		NIST Webbook
tb	815.80	K	Joback Method
tc	1005.36	K	Joback Method
tf	437.47	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.87	J/mol×K	815.80	Joback Method
cpg	1057.35	J/mol×K	847.39	Joback Method
cpg	1075.76	J/mol×K	878.99	Joback Method
cpg	1093.12	J/mol×K	910.58	Joback Method
cpg	1109.51	J/mol×K	942.18	Joback Method
cpg	1124.95	J/mol×K	973.77	Joback Method
cpg	1139.51	J/mol×K	1005.36	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=R519585&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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