3-Methyl-3-sulfanylbutyl Octadecanoate

Inchi: InChI=1S/C23H46O2S/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(24)25-21-20-2
InchiKey: SYRREHCYQUGIRS-UHFFFAOYSA-N
Formula: C23H46O2S
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 386.68

Physical Properties

Property code	Value	Unit	Source
gf	-58.91	kJ/mol	Joback Method
hf	-733.12	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	81.39	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	7.890		Crippen Method
mcvol	358.720	ml/mol	McGowan Method
pc	919.95	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	861.56	K	Joback Method
tc	1056.41	K	Joback Method
tf	460.01	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.07	J/mol×K	861.56	Joback Method
cpg	1182.25	J/mol×K	894.04	Joback Method
cpg	1201.26	J/mol×K	926.51	Joback Method
cpg	1219.16	J/mol×K	958.99	Joback Method
cpg	1236.01	J/mol×K	991.46	Joback Method
cpg	1251.88	J/mol×K	1023.94	Joback Method
cpg	1266.80	J/mol×K	1056.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519609&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

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