3-Methyl-3-sulfanylbutyl Dodecanoate

Inchi: InChI=1S/C17H34O2S/c1-4-5-6-7-8-9-10-11-12-13-16(18)19-15-14-17(2,3)20/h20H,4-15
InchiKey: WUIHIVJGQGIMMG-UHFFFAOYSA-N
Formula: C17H34O2S
SMILES: CCCCCCCCCCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 302.52

Physical Properties

Property code	Value	Unit	Source
gf	-109.43	kJ/mol	Joback Method
hf	-609.28	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	68.03	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.549		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2082.00		NIST Webbook
ripol	2557.00		NIST Webbook
tb	724.28	K	Joback Method
tc	911.43	K	Joback Method
tf	392.39	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.37	J/mol×K	724.28	Joback Method
cpg	817.72	J/mol×K	755.47	Joback Method
cpg	835.10	J/mol×K	786.66	Joback Method
cpg	851.53	J/mol×K	817.85	Joback Method
cpg	867.07	J/mol×K	849.05	Joback Method
cpg	881.74	J/mol×K	880.24	Joback Method
cpg	895.59	J/mol×K	911.43	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=R519570&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume