3-Methyl-3-sulfanylbutyl Decanoate

Inchi: InChI=1S/C15H30O2S/c1-4-5-6-7-8-9-10-11-14(16)17-13-12-15(2,3)18/h18H,4-13H2,1-3
InchiKey: OYXFZHVGAWREDG-UHFFFAOYSA-N
Formula: C15H30O2S
SMILES: CCCCCCCCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 274.46

Physical Properties

Property code	Value	Unit	Source
gf	-126.27	kJ/mol	Joback Method
hf	-568.00	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	63.58	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.769		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
ripol	2342.00		NIST Webbook
tb	678.52	K	Joback Method
tc	867.69	K	Joback Method
tf	369.85	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.15	J/mol×K	678.52	Joback Method
cpg	703.90	J/mol×K	710.05	Joback Method
cpg	720.71	J/mol×K	741.58	Joback Method
cpg	736.62	J/mol×K	773.10	Joback Method
cpg	751.66	J/mol×K	804.63	Joback Method
cpg	765.86	J/mol×K	836.16	Joback Method
cpg	779.27	J/mol×K	867.69	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=R519565&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