3-Methyl-3-sulfanylbutyl Octanoate

Inchi: InChI=1S/C13H26O2S/c1-4-5-6-7-8-9-12(14)15-11-10-13(2,3)16/h16H,4-11H2,1-3H3
InchiKey: XARZJEWJXORBQZ-UHFFFAOYSA-N
Formula: C13H26O2S
SMILES: CCCCCCCC(=O)OCCC(C)(C)S
Mol. weight [g/mol]: 246.41

Physical Properties

Property code	Value	Unit	Source
gf	-143.11	kJ/mol	Joback Method
hf	-526.72	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.989		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1678.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2130.00		NIST Webbook
tb	632.76	K	Joback Method
tc	825.57	K	Joback Method
tf	347.31	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.78	J/mol×K	632.76	Joback Method
cpg	594.78	J/mol×K	664.90	Joback Method
cpg	610.87	J/mol×K	697.03	Joback Method
cpg	626.10	J/mol×K	729.17	Joback Method
cpg	640.49	J/mol×K	761.30	Joback Method
cpg	654.09	J/mol×K	793.44	Joback Method
cpg	666.90	J/mol×K	825.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519614&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume