3-Sulfanylhexyl Decanoate

Inchi: InChI=1S/C16H32O2S/c1-3-5-6-7-8-9-10-12-16(17)18-14-13-15(19)11-4-2/h15,19H,3-14
InchiKey: NILAQKBTIHPRCL-UHFFFAOYSA-N
Formula: C16H32O2S
SMILES: CCCCCCCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 288.49

Physical Properties

Property code	Value	Unit	Source
gf	-123.13	kJ/mol	Joback Method
hf	-585.17	kJ/mol	Joback Method
hfus	40.50	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	5.159		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2003.00		NIST Webbook
ripol	2480.00		NIST Webbook
tb	704.19	K	Joback Method
tc	887.63	K	Joback Method
tf	363.70	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.51	J/mol×K	704.19	Joback Method
cpg	758.38	J/mol×K	734.76	Joback Method
cpg	775.36	J/mol×K	765.34	Joback Method
cpg	791.47	J/mol×K	795.91	Joback Method
cpg	806.73	J/mol×K	826.48	Joback Method
cpg	821.16	J/mol×K	857.06	Joback Method
cpg	834.77	J/mol×K	887.63	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=R519634&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