3-Sulfanylhexyl Dodecanoate

Inchi: InChI=1S/C18H36O2S/c1-3-5-6-7-8-9-10-11-12-14-18(19)20-16-15-17(21)13-4-2/h17,21
InchiKey: WTIXFZHNOBZELM-UHFFFAOYSA-N
Formula: C18H36O2S
SMILES: CCCCCCCCCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 316.54

Physical Properties

Property code	Value	Unit	Source
gf	-106.29	kJ/mol	Joback Method
hf	-626.45	kJ/mol	Joback Method
hfus	45.68	kJ/mol	Joback Method
hvap	71.17	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.939		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpol	2208.00		NIST Webbook
ripol	2696.00		NIST Webbook
tb	749.95	K	Joback Method
tc	933.37	K	Joback Method
tf	386.24	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.45	J/mol×K	749.95	Joback Method
cpg	874.98	J/mol×K	780.52	Joback Method
cpg	892.56	J/mol×K	811.09	Joback Method
cpg	909.21	J/mol×K	841.66	Joback Method
cpg	924.94	J/mol×K	872.23	Joback Method
cpg	939.78	J/mol×K	902.80	Joback Method
cpg	953.77	J/mol×K	933.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519649&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