3-Sulfanylhexyl Octanoate

Inchi: InChI=1S/C14H28O2S/c1-3-5-6-7-8-10-14(15)16-12-11-13(17)9-4-2/h13,17H,3-12H2,1-2
InchiKey: VVATXCLGPZNOEX-UHFFFAOYSA-N
Formula: C14H28O2S
SMILES: CCCCCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 260.44

Physical Properties

Property code	Value	Unit	Source
gf	-139.97	kJ/mol	Joback Method
hf	-543.89	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.379		Crippen Method
mcvol	231.910	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
ripol	2271.00		NIST Webbook
tb	658.43	K	Joback Method
tc	843.79	K	Joback Method
tf	341.16	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.14	J/mol×K	658.43	Joback Method
cpg	646.24	J/mol×K	689.32	Joback Method
cpg	662.51	J/mol×K	720.22	Joback Method
cpg	677.97	J/mol×K	751.11	Joback Method
cpg	692.64	J/mol×K	782.00	Joback Method
cpg	706.53	J/mol×K	812.90	Joback Method
cpg	719.66	J/mol×K	843.79	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519654&Units=SI

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