S-Propylhexadecanthioate

Inchi: InChI=1S/C19H38OS/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19(20)21-18-4-2/h3-18H2
InchiKey: DDWFINHOUDVUAO-UHFFFAOYSA-N
Formula: C19H38OS
SMILES: CCCCCCCCCCCCCCCC(=O)SCCC
Mol. weight [g/mol]: 314.57

Physical Properties

Property code	Value	Unit	Source
gf	13.30	kJ/mol	Joback Method
hf	-506.20	kJ/mol	Joback Method
hfus	50.70	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	7.138		Crippen Method
mcvol	296.490	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	756.77	K	Joback Method
tc	938.45	K	Joback Method
tf	388.22	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.69	J/mol×K	756.77	Joback Method
cpg	907.65	J/mol×K	787.05	Joback Method
cpg	925.63	J/mol×K	817.33	Joback Method
cpg	942.67	J/mol×K	847.61	Joback Method
cpg	958.79	J/mol×K	877.89	Joback Method
cpg	974.03	J/mol×K	908.17	Joback Method
cpg	988.42	J/mol×K	938.45	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=R391174&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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