2,4-Bis(isopentylthio)but-2-enal

Inchi: InChI=1S/C14H26OS2/c1-12(2)5-8-16-9-7-14(11-15)17-10-6-13(3)4/h7,11-13H,5-6,8-10H
InchiKey: SIJYUHKHBDTLPC-AUWJEWJLSA-N
Formula: C14H26OS2
SMILES: CC(C)CCSCC=C(C=O)SCCC(C)C
Mol. weight [g/mol]: 274.49

Physical Properties

Property code	Value	Unit	Source
gf	100.51	kJ/mol	Joback Method
hf	-237.26	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.628		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
ripol	2523.00		NIST Webbook
ripol	2523.00		NIST Webbook
tb	709.10	K	Joback Method
tc	918.94	K	Joback Method
tf	309.30	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.44	J/mol×K	709.10	Joback Method
cpg	661.26	J/mol×K	744.07	Joback Method
cpg	677.07	J/mol×K	779.05	Joback Method
cpg	691.89	J/mol×K	814.02	Joback Method
cpg	705.77	J/mol×K	848.99	Joback Method
cpg	718.75	J/mol×K	883.97	Joback Method
cpg	730.85	J/mol×K	918.94	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=R402016&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume