2,4-Bis(pentylthio)bute-2-nal

Inchi: InChI=1S/C14H26OS2/c1-3-5-7-10-16-12-9-14(13-15)17-11-8-6-4-2/h9,13H,3-8,10-12H2
InchiKey: SSWJNUUBNWGTQY-ZROIWOOFSA-N
Formula: C14H26OS2
SMILES: CCCCCSCC=C(C=O)SCCCCC
Mol. weight [g/mol]: 274.49

Physical Properties

Property code	Value	Unit	Source
gf	105.39	kJ/mol	Joback Method
hf	-226.70	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.916		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
ripol	2740.00		NIST Webbook
ripol	2740.00		NIST Webbook
tb	709.98	K	Joback Method
tc	912.99	K	Joback Method
tf	339.30	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.41	J/mol×K	709.98	Joback Method
cpg	659.65	J/mol×K	743.82	Joback Method
cpg	674.95	J/mol×K	777.65	Joback Method
cpg	689.35	J/mol×K	811.49	Joback Method
cpg	702.89	J/mol×K	845.32	Joback Method
cpg	715.60	J/mol×K	879.16	Joback Method
cpg	727.50	J/mol×K	912.99	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=R402041&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