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

Inchi: InChI=1S/C12H22OS2/c1-10(2)8-14-6-5-12(7-13)15-9-11(3)4/h5,7,10-11H,6,8-9H2,1-4H
InchiKey: CTBYEASLMKFJPI-XGICHPGQSA-N
Formula: C12H22OS2
SMILES: CC(C)CSCC=C(C=O)SCC(C)C
Mol. weight [g/mol]: 246.43

Physical Properties

Property code	Value	Unit	Source
gf	83.67	kJ/mol	Joback Method
hf	-195.98	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.848		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
ripol	2302.00		NIST Webbook
ripol	2302.00		NIST Webbook
tb	663.34	K	Joback Method
tc	879.58	K	Joback Method
tf	286.76	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.53	J/mol×K	663.34	Joback Method
cpg	553.59	J/mol×K	699.38	Joback Method
cpg	568.66	J/mol×K	735.42	Joback Method
cpg	582.79	J/mol×K	771.46	Joback Method
cpg	596.00	J/mol×K	807.50	Joback Method
cpg	608.34	J/mol×K	843.54	Joback Method
cpg	619.84	J/mol×K	879.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R402001&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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