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

Inchi: InChI=1S/C10H18OS2/c1-8(2)12-6-5-10(7-11)13-9(3)4/h5,7-9H,6H2,1-4H3/b10-5-
InchiKey: ZDPDFFMZPRJHCR-YHYXMXQVSA-N
Formula: C10H18OS2
SMILES: CC(C)SCC=C(C=O)SC(C)C
Mol. weight [g/mol]: 218.38

Physical Properties

Property code	Value	Unit	Source
gf	66.83	kJ/mol	Joback Method
hf	-154.70	kJ/mol	Joback Method
hfus	24.05	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.352		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
ripol	2176.00		NIST Webbook
ripol	2176.00		NIST Webbook
tb	617.58	K	Joback Method
tc	841.61	K	Joback Method
tf	264.22	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.05	J/mol×K	617.58	Joback Method
cpg	451.00	J/mol×K	654.92	Joback Method
cpg	465.03	J/mol×K	692.26	Joback Method
cpg	478.16	J/mol×K	729.60	Joback Method
cpg	490.42	J/mol×K	766.94	Joback Method
cpg	501.86	J/mol×K	804.27	Joback Method
cpg	512.50	J/mol×K	841.61	Joback Method

Sources

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=R402021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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