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

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

Physical Properties

Property code	Value	Unit	Source
gf	71.71	kJ/mol	Joback Method
hf	-144.14	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.356		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
ripol	2225.00		NIST Webbook
ripol	2225.00		NIST Webbook
tb	618.46	K	Joback Method
tc	833.50	K	Joback Method
tf	294.22	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.14	J/mol×K	618.46	Joback Method
cpg	449.40	J/mol×K	654.30	Joback Method
cpg	462.82	J/mol×K	690.14	Joback Method
cpg	475.45	J/mol×K	725.98	Joback Method
cpg	487.29	J/mol×K	761.82	Joback Method
cpg	498.39	J/mol×K	797.66	Joback Method
cpg	508.77	J/mol×K	833.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R402061&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