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

Inchi: InChI=1S/C16H30OS2/c1-3-5-7-9-12-18-14-11-16(15-17)19-13-10-8-6-4-2/h11,15H,3-10
InchiKey: FVAYBXDMKZUFRV-WJDWOHSUSA-N
Formula: C16H30OS2
SMILES: CCCCCCSCC=C(C=O)SCCCCCC
Mol. weight [g/mol]: 302.54

Physical Properties

Property code	Value	Unit	Source
gf	122.23	kJ/mol	Joback Method
hf	-267.98	kJ/mol	Joback Method
hfus	46.64	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.696		Crippen Method
mcvol	266.270	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
ripol	2877.00		NIST Webbook
ripol	2877.00		NIST Webbook
tb	755.74	K	Joback Method
tc	955.21	K	Joback Method
tf	361.84	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.05	J/mol×K	755.74	Joback Method
cpg	771.92	J/mol×K	788.99	Joback Method
cpg	787.82	J/mol×K	822.23	Joback Method
cpg	802.79	J/mol×K	855.48	Joback Method
cpg	816.85	J/mol×K	888.72	Joback Method
cpg	830.06	J/mol×K	921.97	Joback Method
cpg	842.44	J/mol×K	955.21	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=R401999&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