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

Inchi: InChI=1S/C10H14OS2/c1-3-6-12-8-5-10(9-11)13-7-4-2/h3-5,9H,1-2,6-8H2/b10-5-
InchiKey: LXRCGXLXWZDREG-YHYXMXQVSA-N
Formula: C10H14OS2
SMILES: C=CCSCC=C(C=O)SCC=C
Mol. weight [g/mol]: 214.35

Physical Properties

Property code	Value	Unit	Source
gf	247.39	kJ/mol	Joback Method
hf	106.72	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	56.91	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.908		Crippen Method
mcvol	173.130	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
ripol	2692.00		NIST Webbook
tb	611.82	K	Joback Method
tc	835.74	K	Joback Method
tf	290.70	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.76	J/mol×K	611.82	Joback Method
cpg	405.64	J/mol×K	649.14	Joback Method
cpg	417.69	J/mol×K	686.46	Joback Method
cpg	428.93	J/mol×K	723.78	Joback Method
cpg	439.42	J/mol×K	761.10	Joback Method
cpg	449.19	J/mol×K	798.42	Joback Method
cpg	458.28	J/mol×K	835.74	Joback Method

Sources

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=R401964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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