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

Inchi: InChI=1S/C6H10OS2/c1-8-4-3-6(5-7)9-2/h3,5H,4H2,1-2H3/b6-3-
InchiKey: MOUMLULBENRQGW-UTCJRWHESA-N
Formula: C6H10OS2
SMILES: CSCC=C(C=O)SC
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	38.03	kJ/mol	Joback Method
hf	-61.58	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	49.34	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.795		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
ripol	1815.00		NIST Webbook
ripol	1815.00		NIST Webbook
tb	526.94	K	Joback Method
tc	758.26	K	Joback Method
tf	249.14	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.64	J/mol×K	526.94	Joback Method
cpg	262.22	J/mol×K	565.49	Joback Method
cpg	272.17	J/mol×K	604.05	Joback Method
cpg	281.51	J/mol×K	642.60	Joback Method
cpg	290.25	J/mol×K	681.15	Joback Method
cpg	298.41	J/mol×K	719.70	Joback Method
cpg	306.01	J/mol×K	758.26	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=R402036&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