Butanal, 2,3-bis-(methylthio)

Inchi: InChI=1S/C6H12OS2/c1-5(8-2)6(4-7)9-3/h4-6H,1-3H3/t5-,6+/m0/s1
InchiKey: MFXACQQJJCSIDY-NTSWFWBYSA-N
Formula: C6H12OS2
SMILES: CSC(C)C(C=O)SC
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	-38.52	kJ/mol	Joback Method
hf	-179.57	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.668		Crippen Method
mcvol	129.670	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1305.00		NIST Webbook
rinpol	1305.00		NIST Webbook
tb	522.02	K	Joback Method
tc	748.63	K	Joback Method
tf	238.18	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.11	J/mol×K	522.02	Joback Method
cpg	282.85	J/mol×K	559.79	Joback Method
cpg	293.97	J/mol×K	597.56	Joback Method
cpg	304.47	J/mol×K	635.33	Joback Method
cpg	314.34	J/mol×K	673.10	Joback Method
cpg	323.59	J/mol×K	710.86	Joback Method
cpg	332.23	J/mol×K	748.63	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=R121712&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume