2-Heptanone, 6-methyl-5,6-bis-(methylthio)

Inchi: InChI=1S/C10H20OS2/c1-8(11)6-7-9(12-4)10(2,3)13-5/h9H,6-7H2,1-5H3
InchiKey: UMXGLMGMLUBWGC-UHFFFAOYSA-N
Formula: C10H20OS2
SMILES: CSC(CCC(C)=O)C(C)(C)SC
Mol. weight [g/mol]: 220.40

Physical Properties

Property code	Value	Unit	Source
gf	-28.96	kJ/mol	Joback Method
hf	-292.60	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	56.55	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.229		Crippen Method
mcvol	186.030	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1596.00		NIST Webbook
tb	615.96	K	Joback Method
tc	840.20	K	Joback Method
tf	308.61	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.43	J/mol×K	615.96	Joback Method
cpg	475.45	J/mol×K	653.33	Joback Method
cpg	490.44	J/mol×K	690.71	Joback Method
cpg	504.43	J/mol×K	728.08	Joback Method
cpg	517.45	J/mol×K	765.45	Joback Method
cpg	529.54	J/mol×K	802.83	Joback Method
cpg	540.75	J/mol×K	840.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121638&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

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