2-Pentanone, 4-methyl-3,4-bis-(methylthio)

Inchi: InChI=1S/C8H16OS2/c1-6(9)7(10-4)8(2,3)11-5/h7H,1-5H3
InchiKey: PIOYFIYKPPYDJV-UHFFFAOYSA-N
Formula: C8H16OS2
SMILES: CSC(C(C)=O)C(C)(C)SC
Mol. weight [g/mol]: 192.34

Physical Properties

Property code	Value	Unit	Source
gf	-45.80	kJ/mol	Joback Method
hf	-251.32	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	52.10	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.449		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1451.00		NIST Webbook
tb	570.20	K	Joback Method
tc	803.31	K	Joback Method
tf	286.07	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.79	J/mol×K	570.20	Joback Method
cpg	377.43	J/mol×K	609.05	Joback Method
cpg	391.11	J/mol×K	647.90	Joback Method
cpg	403.84	J/mol×K	686.76	Joback Method
cpg	415.68	J/mol×K	725.61	Joback Method
cpg	426.64	J/mol×K	764.46	Joback Method
cpg	436.76	J/mol×K	803.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121643&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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