2-[(1-methyl-2-oxopropyl)-thio]-3-pentanone

Inchi: InChI=1S/C9H16O2S/c1-5-9(11)8(4)12-7(3)6(2)10/h7-8H,5H2,1-4H3
InchiKey: AODKKQZCGLPMNH-UHFFFAOYSA-N
Formula: C9H16O2S
SMILES: CCC(=O)C(C)SC(C)C(C)=O
Mol. weight [g/mol]: 188.29

Physical Properties

Property code	Value	Unit	Source
gf	-204.70	kJ/mol	Joback Method
hf	-422.94	kJ/mol	Joback Method
hfus	19.35	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.065		Crippen Method
mcvol	157.160	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
tb	580.96	K	Joback Method
tc	790.72	K	Joback Method
tf	295.45	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.17	J/mol×K	580.96	Joback Method
cpg	385.79	J/mol×K	615.92	Joback Method
cpg	398.67	J/mol×K	650.88	Joback Method
cpg	410.82	J/mol×K	685.84	Joback Method
cpg	422.26	J/mol×K	720.80	Joback Method
cpg	432.99	J/mol×K	755.76	Joback Method
cpg	443.02	J/mol×K	790.72	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=R222989&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