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

Inchi: InChI=1S/C9H16O2S3/c1-5-9(11)8(4)13-14-12-7(3)6(2)10/h7-8H,5H2,1-4H3
InchiKey: MCCKMSMZABNXEW-UHFFFAOYSA-N
Formula: C9H16O2S3
SMILES: CCC(=O)C(C)SSSC(C)C(C)=O
Mol. weight [g/mol]: 252.42

Physical Properties

Property code	Value	Unit	Source
gf	-138.46	kJ/mol	Joback Method
hf	-339.20	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	68.80	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.361		Crippen Method
mcvol	189.860	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	718.52	K	Joback Method
tc	960.85	K	Joback Method
tf	364.25	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.70	J/mol×K	718.52	Joback Method
cpg	486.78	J/mol×K	758.91	Joback Method
cpg	498.79	J/mol×K	799.30	Joback Method
cpg	509.73	J/mol×K	839.69	Joback Method
cpg	519.59	J/mol×K	880.07	Joback Method
cpg	528.38	J/mol×K	920.46	Joback Method
cpg	536.09	J/mol×K	960.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222994&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