2-(1-Methyl-2-oxopropyldithio)pentan-3-one, #2

Inchi: InChI=1S/C9H16O2S2/c1-5-9(11)8(4)13-12-7(3)6(2)10/h7-8H,5H2,1-4H3
InchiKey: DYAXZUZAGRJLCX-UHFFFAOYSA-N
Formula: C9H16O2S2
SMILES: CCC(=O)C(C)SSC(C)C(C)=O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	-171.58	kJ/mol	Joback Method
hf	-381.07	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	61.98	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.713		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	649.74	K	Joback Method
tc	876.37	K	Joback Method
tf	329.85	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.62	J/mol×K	649.74	Joback Method
cpg	437.16	J/mol×K	687.51	Joback Method
cpg	449.82	J/mol×K	725.28	Joback Method
cpg	461.60	J/mol×K	763.05	Joback Method
cpg	472.51	J/mol×K	800.83	Joback Method
cpg	482.56	J/mol×K	838.60	Joback Method
cpg	491.75	J/mol×K	876.37	Joback Method

Sources

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=R90448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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