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

Other names: 2-(1-Methyl-2-oxopropyldithio)pentan-3-one, #1
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]: 220.36

Physical Properties

Property code	Value	Unit	Source
hf	-464.76	kJ/mol	Cheméo Relay (1.0)
hfus	23.48	kJ/mol	Joback Method
hvap	66.05	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-1.62		Cheméo Relay (1.0)
logp	2.713		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
tb	534.05	K	Cheméo Relay (1.0)
tc	740.09	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R90484

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature