3-[(1-methyl-2-oxobutyl)-dithio]-2-pentanone

Inchi: InChI=1S/C10H18O2S2/c1-5-9(12)8(4)13-14-10(6-2)7(3)11/h8,10H,5-6H2,1-4H3
InchiKey: XXXOWSFREAVVBG-UHFFFAOYSA-N
Formula: C10H18O2S2
SMILES: CCC(=O)C(C)SSC(CC)C(C)=O
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	-163.16	kJ/mol	Joback Method
hf	-401.71	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	64.20	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.103		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	672.62	K	Joback Method
tc	895.13	K	Joback Method
tf	341.12	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.93	J/mol×K	672.62	Joback Method
cpg	488.07	J/mol×K	709.70	Joback Method
cpg	501.29	J/mol×K	746.79	Joback Method
cpg	513.59	J/mol×K	783.87	Joback Method
cpg	524.98	J/mol×K	820.96	Joback Method
cpg	535.47	J/mol×K	858.04	Joback Method
cpg	545.08	J/mol×K	895.13	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=R222949&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