

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

Other names:	2-oxo-3-pentyl 3-oxo-2-butyl disulfide 3-(1-Methyl-2-oxopropyl)dithio)pentan-2-one
Inchi:	InChI=1S/C9H16O2S2/c1-5-9(7(3)11)13-12-8(4)6(2)10/h8-9H,5H2,1-4H3
InchiKey:	OXSWG HQNGIZSSA-UHFFFAOYSA-N
Formula:	C9H16O2S2
SMILES:	CCC(SSC(C)C(C)=O)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	1532.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1539.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2227.00		NIST Webbook
tb	649.74	K	Joback Method
tc	876.37	K	Joback Method
tf	329.85	K	Joback Method
vc	0.647	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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=R90569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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