

2-Butanone, 4-(2,2-dimethyl-6-methylenecyclohexyl)-

Other names:	4-(2,2-Dimethyl-6-methylenecyclohexyl)-2-butanone 4-(2,2-dimethyl-6-methylenecyclohexyl)butan-2-one
Inchi:	InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h12H,1,5-9H2,2-4H3
InchiKey:	ZLPHULOLXDKCND-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	C=C1CCCC(C)(C)C1CCC(C)=O
Mol. weight [g/mol]:	194.31
CAS:	13720-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-6.01	kJ/mol	Joback Method
hf	-290.77	kJ/mol	Joback Method
hfus	16.47	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.738		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1396.30		NIST Webbook
rinpol	1396.30		NIST Webbook
rinpol	1417.00		NIST Webbook
ripol	1798.00		NIST Webbook
tb	564.99	K	Joback Method
tc	772.57	K	Joback Method
tf	326.92	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.25	J/mol×K	564.99	Joback Method
cpg	475.48	J/mol×K	599.59	Joback Method
cpg	493.66	J/mol×K	634.18	Joback Method

cpg	510.89	J/mol×K	668.78	Joback Method
cpg	527.26	J/mol×K	703.38	Joback Method
cpg	542.86	J/mol×K	737.98	Joback Method
cpg	557.80	J/mol×K	772.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13720122&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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