2-Butanone, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-

Other names: 4-(2,2,6-Trimethyl-5-cyclohexen-1-yl)-2-butanone
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-butanone
Dihydro-«alpha»-ionone
2',2''-Dihydro-«alpha»-ionone
«alpha»-Dihydroionone
«alpha»-7,8-Dihydroionone
7,8-Dihydro-.alpha.-ionone
49749-39-5
4-(2,6,6-trimethyl-2-cyclohexen-1-yl)butan-2-one

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6,12H,5,7-9H2,1-4H3

InchiKey: JHJCHCSUEGPIGE-UHFFFAOYSA-N

Formula: C13H22O

SMILES: CC(=O)CCC1C(C)=CCCC1(C)C

Mol. weight [g/mol]: 194.31

CAS: 31499-72-6

Physical Properties

Property code	Value	Unit	Source
gf	-38.76	kJ/mol	Joback Method
hf	-328.70	kJ/mol	Joback Method
hfus	18.47	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.738		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1406.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1437.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1854.00		NIST Webbook
tb	569.97	K	Joback Method
tc	778.76	K	Joback Method
tf	326.52	K	Joback Method

vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.48	J/mol×K	569.97	Joback Method
cpg	476.52	J/mol×K	604.77	Joback Method
cpg	494.51	J/mol×K	639.57	Joback Method
cpg	511.57	J/mol×K	674.37	Joback Method
cpg	527.78	J/mol×K	709.16	Joback Method
cpg	543.25	J/mol×K	743.96	Joback Method
cpg	558.07	J/mol×K	778.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31499726&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