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

Other names: «alpha»,«beta»-Dihydro-«beta»-ionone
«beta»-Ionone, dihydro-
Dihydro-«beta»-ionone
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone
4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanone
7,8-Dihydro-«beta»-ionone
1-(1,1,5-Trimethylcyclohex-5-en-6-yl)-butan-3-one
«beta»-7,8-Dihydroionone
7,8-dehydro-«beta»-ionone
4-(2,6,6-trimethyl-1-cyclohexen-1-yl)butan-2-one
4-(1,1,5-Trimethylcyclohex-5-en-6-yl)-butan-3-one

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-9H2,1-4H3

InchiKey: QJJDNZGPQDGNDX-UHFFFAOYSA-N

Formula: C13H22O

SMILES: CC(=O)CCC1=C(C)CCCC1(C)C

Mol. weight [g/mol]: 194.31

CAS: 17283-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-40.68	kJ/mol	Joback Method
hf	-319.83	kJ/mol	Joback Method
hfus	17.01	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.882		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1414.00		NIST Webbook
ripol	1849.00		NIST Webbook
tb	579.62	K	Joback Method
tc	789.51	K	Joback Method
tf	343.28	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.66	J/mol×K	579.62	Joback Method
cpg	474.94	J/mol×K	614.60	Joback Method
cpg	492.25	J/mol×K	649.58	Joback Method
cpg	508.68	J/mol×K	684.57	Joback Method
cpg	524.34	J/mol×K	719.55	Joback Method
cpg	539.31	J/mol×K	754.53	Joback Method
cpg	553.72	J/mol×K	789.51	Joback Method

Sources

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=C17283817&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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