2-Butanone, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-

Other names: 4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)butan-2-one
4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanone
4-(2,6,6-trimethyl cyclohexa-1,3-dienyl) butane-2-one
Dihydrodehydro-«beta»-ionone
7,8-Dihydro-3,4-dehydro-«beta»-ionone
iso-«beta»-ionone 4(2,6,6-trimethyl-1,3,cyclo-hexadienyl) butan-2-one
3,4-didehydro-7,8-dihydro-«beta»-ionone
4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)butan-2-one

Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-6H,7-9H2,1-4H3

InchiKey: SQFRYZPEWOZAKJ-UHFFFAOYSA-N

Formula: C13H20O

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

Mol. weight [g/mol]: 192.30

CAS: 20483-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-10.72	kJ/mol	Joback Method
hf	-262.05	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	52.46	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1425.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
ripol	1841.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1865.00		NIST Webbook
tb	578.78	K	Joback Method
tc	790.61	K	Joback Method
tf	344.04	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.65	J/mol×K	578.78	Joback Method
cpg	453.84	J/mol×K	614.09	Joback Method
cpg	470.09	J/mol×K	649.39	Joback Method
cpg	485.49	J/mol×K	684.70	Joback Method
cpg	500.16	J/mol×K	720.00	Joback Method
cpg	514.19	J/mol×K	755.31	Joback Method
cpg	527.70	J/mol×K	790.61	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20483367&Units=SI

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