«alpha»-Ionone

Other names:	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-
	«alpha»-Cyclocitrylideneacetone
	(E)-«alpha»-Ionone
	trans-«alpha»-Ionone
	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, trans
	4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, (E)-
	(3E)-4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
	«alpha»-(E)-Ionone
	trans-4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (3E)-
	4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one («alpha»-ionone)
	4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
	4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one
	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-(.+/-.)-
Inchi:	InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6-8,12H,5,9H2,1-4H3/b8-7+
InchiKey:	UZFLPKAIBPNNCA-BQYQJAHWSA-N
Formula:	C13H20O
SMILES:	CC(=O)C=CC1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	192.30
CAS:	30685-95-1

Physical Properties

Property code	Value	Unit	Source
chl	-7697.30	kJ/mol	NIST Webbook
gf	41.46	kJ/mol	Joback Method
hf	-211.48	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	51.16	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
tb	574.13	K	Joback Method
tc	792.17	K	Joback Method
tf	321.44	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.46	J/mol×K	574.13	Joback Method
cpg	457.12	J/mol×K	610.47	Joback Method
cpg	474.66	J/mol×K	646.81	Joback Method
cpg	491.22	J/mol×K	683.15	Joback Method
cpg	506.92	J/mol×K	719.49	Joback Method
cpg	521.90	J/mol×K	755.83	Joback Method
cpg	536.27	J/mol×K	792.17	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30685951&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

Legend

chl: Standard liquid enthalpy of combustion
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume