3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

Other names: 4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-buten-2-one
«beta»-Ionone
«beta»-Cyclocitrylideneacetone
Ionone, «beta»-
4-(2,6,6-Trimethyl-1-cyclohexen-l-yl)-3-buten-2-one
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
4-(2,6,6-trimethyl-1-cyclohexene-1-yl)-3-buten-2-one
4-(2,6,6-Trimethylcyclohex-1-en-1-yl)but-3-en-2-one
NSC 402758
4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one («beta»-ionone)
«beta»-Ionene
4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one

Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8H,5-6,9H2,1-4H3/b8-7+

InchiKey: PSQYTAPXSHCGMF-BQYQJAHWSA-N

Formula: C13H20O

SMILES: CC(=O)C=CC1=C(C)CCCC1(C)C

Mol. weight [g/mol]: 192.30

CAS: 14901-07-6

Physical Properties

Property code	Value	Unit	Source
chl	-7760.50 ± 2.80	kJ/mol	NIST Webbook
gf	39.54	kJ/mol	Joback Method
hf	-202.61	kJ/mol	Joback Method
hfl	-213.40 ± 2.80	kJ/mol	NIST Webbook
hfus	17.21	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1488.40		NIST Webbook
rinpol	1486.00		NIST Webbook

rinpol	1493.00		NIST Webbook
rinpol	1496.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1986.00		NIST Webbook
tb	583.78	K	Joback Method
tc	802.88	K	Joback Method
tf	338.20	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.51	J/mol×K	766.36	Joback Method
cpg	437.25	J/mol×K	583.78	Joback Method
cpg	455.12	J/mol×K	620.30	Joback Method
cpg	471.95	J/mol×K	656.81	Joback Method
cpg	487.87	J/mol×K	693.33	Joback Method
cpg	503.02	J/mol×K	729.85	Joback Method
cpg	531.49	J/mol×K	802.88	Joback Method
hvapt	69.00	kJ/mol	312.50	NIST Webbook

Sources

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=C14901076&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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