3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-

Other names: «beta»-Irone
6-Methyl-«beta»-ionone
«beta»-Methylionone
2-Methyl-«beta»-ionone
beta-Irone
«beta»-Ionone, 6-methyl-
NSC 402758
4-(2,6,6-Trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one
4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-3-buten-2-one

Inchi: InChI=1S/C14H22O/c1-10-6-7-11(2)14(4,5)13(10)9-8-12(3)15/h8-9,11H,6-7H2,1-5H3/b9-

InchiKey: BGKCUGPVLVNPSG-CMDGGOBGSA-N

Formula: C14H22O

SMILES: CC(=O)C=CC1=C(C)CCC(C)C1(C)C

Mol. weight [g/mol]: 206.32

CAS: 79-70-9

Physical Properties

Property code	Value	Unit	Source
gf	40.25	kJ/mol	Joback Method
hf	-243.59	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	54.05	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1583.40		NIST Webbook
tb	601.99	K	Joback Method
tc	817.25	K	Joback Method
tf	345.23	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.38	J/mol×K	601.99	Joback Method
cpg	508.25	J/mol×K	637.87	Joback Method
cpg	526.10	J/mol×K	673.74	Joback Method
cpg	543.05	J/mol×K	709.62	Joback Method
cpg	559.21	J/mol×K	745.50	Joback Method
cpg	574.71	J/mol×K	781.37	Joback Method
cpg	589.67	J/mol×K	817.25	Joback Method
hvapt	72.10	kJ/mol	310.50	NIST Webbook

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=C79709&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume