«gamma»-Irone

Other names: 6-Methyl- «gamma»-(E)-ionone
4-(2,2,3-trimethyl-6-methylenecyclohexyl)-3-buten-2-one
4-(2,2,3-trimethyl-6-methylenecyclohexyl)but-3-en-2-one
Inchi: InChI=1S/C14H22O/c1-10-6-7-11(2)14(4,5)13(10)9-8-12(3)15/h8-9,11,13H,1,6-7H2,2-5H
InchiKey: MVPDTCQYNRKWJA-CMDGGOBGSA-N
Formula: C14H22O
SMILES: C=C1CCC(C)C(C)(C)C1C=CC(C)=O
Mol. weight [g/mol]: 206.32
CAS: 79-68-5

Physical Properties

Property code	Value	Unit	Source
gf	74.92	kJ/mol	Joback Method
hf	-214.53	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	52.28	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.760		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1561.90		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1561.90		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1476.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1834.00		NIST Webbook
tb	587.36	K	Joback Method
tc	800.43	K	Joback Method
tf	328.87	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.39	J/mol×K	587.36	Joback Method
cpg	509.20	J/mol×K	622.87	Joback Method
cpg	527.92	J/mol×K	658.38	Joback Method
cpg	545.64	J/mol×K	693.90	Joback Method
cpg	562.49	J/mol×K	729.41	Joback Method
cpg	578.58	J/mol×K	764.92	Joback Method
cpg	594.01	J/mol×K	800.43	Joback Method

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=C79685&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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