Cyclohexanone, 5-ethenyl-5-methyl-4-(1-methylethenyl)-2-(1-methy
cis-

Other names: c-«beta»-Elemenone
cis-«beta»-Elemenone
Cyclohexanone, 5-ethenyl-5-methyl-4-(1-methylethenyl)-2-(1-methylethylidene)-, (4R,5S)-rel-
4-Isopropenyl-5-methyl-2-(1-methylethylidene)-5-vinylcyclohexanone, cis

Inchi: InChI=1S/C15H22O/c1-7-15(6)9-14(16)12(10(2)3)8-13(15)11(4)5/h7,13H,1,4,8-9H2,2-3,5

InchiKey: ABLPGPHZENVRRH-UKRRQHHQSA-N

Formula: C15H22O

SMILES: C=CC1(C)CC(=O)C(=C(C)C)CC1C(=C)C

Mol. weight [g/mol]: 218.33

CAS: 32663-57-3

Physical Properties

Property code	Value	Unit	Source
gf	168.12	kJ/mol	Joback Method
hf	-134.10	kJ/mol	Joback Method
hfus	15.87	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.070		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1597.00		NIST Webbook
ripol	2070.00		NIST Webbook
tb	625.30	K	Joback Method
tc	852.13	K	Joback Method
tf	332.99	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.91	J/mol×K	625.30	Joback Method
cpg	550.52	J/mol×K	663.11	Joback Method
cpg	570.03	J/mol×K	700.91	Joback Method
cpg	588.56	J/mol×K	738.72	Joback Method
cpg	606.24	J/mol×K	776.52	Joback Method
cpg	623.19	J/mol×K	814.33	Joback Method
cpg	639.53	J/mol×K	852.13	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32663573&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

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