«beta»-Elemenone

Other names:	(4S)--trans-«beta»-Elemenone Cyclohexanone, 5-ethenyl-5-methyl-4-(1-methylethenyl)-2-(1-methylethylidene)-, (4S,5S)- 4-Isopropenyl-5-methyl-2-(1-methylethylidene)-5-vinylcyclohexanone, (4S,5S)- Cyclohexanone, 5-ethenyl-5-methyl-4-(1-methylethenyl)-2-(1-methylethylidene)-, (4S-trans)- elemenone
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-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	C=CC1(C)CC(=O)C(=C(C)C)CC1C(=C)C
Mol. weight [g/mol]:	218.33
CAS:	20303-60-0

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	1605.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1606.50		NIST Webbook
ripol	2099.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2091.00		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

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=C20303600&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