2-Cyclohexen-1-one, 2-hydroxy-3-methyl-6-(1-methylethyl)-

Other names: Diosphenol
Barosma camphor
Buccocamphor
Buchu camphor
2-Hydroxypiperitone
2-hydroxy-6-(isopropyl)-3-methylcyclohex-2-en-1-one

Inchi: InChI=1S/C10H16O2/c1-6(2)8-5-4-7(3)9(11)10(8)12/h6,8,11H,4-5H2,1-3H3

InchiKey: QSIMLPCPCXVYDD-UHFFFAOYSA-N

Formula: C10H16O2

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

Mol. weight [g/mol]: 168.23

CAS: 490-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-193.38	kJ/mol	Joback Method
hf	-455.78	kJ/mol	Joback Method
hfus	14.01	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.454		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1304.90		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1304.90		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1273.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1830.00		NIST Webbook

tb	616.43	K	Joback Method
tc	823.06	K	Joback Method
tf	349.68	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.65	J/mol×K	616.43	Joback Method
cpg	395.28	J/mol×K	650.87	Joback Method
cpg	409.19	J/mol×K	685.31	Joback Method
cpg	422.36	J/mol×K	719.75	Joback Method
cpg	434.79	J/mol×K	754.19	Joback Method
cpg	446.47	J/mol×K	788.62	Joback Method
cpg	457.40	J/mol×K	823.06	Joback Method
hvapt	56.20	kJ/mol	422.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C490039&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
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