

Carvone

Other names:	(-)-carvone (.+/-)-Carvone (R)-Carvone (Z)-dihydrocarvone 1(6),8-p-Menthadien-2-one 1-Carvone 2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- 2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one 2-Methyl-5-(1-methylethenyl)-2-cyclohexene-1-one 2-Methyl-5-isopropenyl-2-cyclohexen-1-one 2-Methyl-5-isopropenyl-2-cyclohexenone 6,8(9)-p-Menthadien-2-one Carvol DL-Carvone Dihydrocarvone Karvon Limonen-6-one NCI-C55867 NSC 6275 R-(-)-carvone cis-Dihydrocarvone d-p-mentha-1(6),8-dien-2-one p-Mentha-6,8-dien-2-one «delta»(6,8)-(9)-Terpadienone-2 Â«deltaÂ»(6,8)-(9)-Terpadienone-2
Inchi:	InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3
InchiKey:	ULDHMXUKGWMISQ-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	<chem>C=C(C)C1CC=C(C)C(=O)C1</chem>
Mol. weight [g/mol]:	150.22
CAS:	99-49-0

Physical Properties

Property code	Value	Unit	Source
gf	34.80	kJ/mol	Joback Method
hf	-171.16	kJ/mol	Joback Method

hfus	11.24		kJ/mol	Joback Method
hvap	42.89		kJ/mol	Joback Method
log10ws	-2.06			Estimated Solubility Method
logp	2.488			Crippen Method
mcvol	133.870		ml/mol	McGowan Method
pc	2859.68		kPa	Joback Method
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ripol	1743.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1750.00		NIST Webbook
tb	502.15 ± 0.50	K	NIST Webbook
tb	504.20 ± 0.50	K	NIST Webbook
tb	504.10 ± 0.50	K	NIST Webbook
tc	742.23	K	Joback Method
tf	275.62	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.34	J/mol×K	516.27	Joback Method
cpg	319.31	J/mol×K	553.93	Joback Method
cpg	335.43	J/mol×K	591.59	Joback Method
cpg	350.72	J/mol×K	629.25	Joback Method
cpg	365.16	J/mol×K	666.91	Joback Method
cpg	378.76	J/mol×K	704.57	Joback Method
cpg	391.51	J/mol×K	742.23	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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