D-Carvone

Other names:	(+)-Carvon (+)-carvone (S)-(+)-carvone (S)-(+)-p-Mentha-6,8-dien-2-one (S)-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one (S)-2-methyl-5-(1-methylvinyl)cyclohex-2-en-1-one (S)-carvone 2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)-, (5S)- 2-cyclohexen-1-one, 2-methyl-5-(1-methylethenyl), (5R)- 2-cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)-, (S)- 5-Isopropenyl-2-methyl-2-cyclohexen-1-one, (S)- D-(+)-carvone R-(-)-1-methyl-4-isopropenyl-6-cyclohexen-2-one carvone, (+)- d-1-Methyl-4-isopropenyl-6-cyclohexen-2-one d-p-Mentha-6,8(9)-dien-2-one l-1-methyl-4-isopropenyl-6-cyclohexen-2-one l-carvone p-mentha-6,8-dien-2-one p-mentha-6,8-dien-2-one, (S)-(+)-
Inchi:	InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3/t9-/m1/s1
InchiKey:	ULDHMXUKGWMISQ-SECBINFHSA-N
Formula:	C10H14O
SMILES:	C=C(C)C1CC=C(C)C(=O)C1
Mol. weight [g/mol]:	150.22
CAS:	2244-16-8

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	58.20	kJ/mol	NIST Webbook
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method

rinpol	1240.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1205.05	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1212.83	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1263.00	NIST Webbook
rinpol	1222.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1212.83	NIST Webbook
rinpol	1216.93	NIST Webbook
rinpol	1221.14	NIST Webbook
rinpol	1225.42	NIST Webbook
rinpol	1229.89	NIST Webbook
rinpol	1234.47	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1194.54	NIST Webbook
rinpol	1197.94	NIST Webbook
rinpol	1201.12	NIST Webbook
rinpol	1205.05	NIST Webbook
rinpol	1208.89	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1234.47	NIST Webbook
ripol	1714.00	NIST Webbook
ripol	1752.00	NIST Webbook
ripol	1715.00	NIST Webbook
ripol	1729.00	NIST Webbook
ripol	1721.00	NIST Webbook
ripol	1741.00	NIST Webbook

ripol	1728.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1745.00		NIST Webbook
tb	504.20	K	NIST Webbook
tc	742.23	K	Joback Method
tf	275.62	K	Joback Method
vc	0.503	m3/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
hfust	1.50	kJ/mol	221.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	1.30	NIST Webbook

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
101.80	298.15	958.79

Reference *https://www.doi.org/10.1016/j.jct.2013.11.026*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2244168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Viscosities and densities of systems involved in the deterpenation of essential oils by liquid–liquid extraction: New UNIFAC-VISCO parameters:	https://www.doi.org/10.1016/j.jct.2013.11.026
High Pressure Phase Equilibria of the Related Substances carvone, limonene and carveol in Supercritical CO2:	https://www.doi.org/10.1021/je020150k
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
hfust:	Enthalpy of fusion at a given temperature
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume