Carvenone

Other names:	2-Cyclohexen-1-one, 6-methyl-3-(1-methylethyl)-
	p-Menth-3-en-2-one
	p-3-menthen-2-one (carvenone)
	3-(isopropyl)-6-methylcyclohex-2-en-1-one
Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h6-8H,4-5H2,1-3H3
InchiKey:	RLYSXAZAJUMULG-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC(C)C1=CC(=O)C(C)CC1
Mol. weight [g/mol]:	152.23
CAS:	499-74-1

Physical Properties

Property code	Value	Unit	Source
chl	-5895.70	kJ/mol	NIST Webbook
gf	-46.93	kJ/mol	Joback Method
hf	-292.08	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	43.10	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1236.20		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1252.00		NIST Webbook

rinpol	1258.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1258.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1737.00		NIST Webbook
tb	519.27	K	Joback Method
tc	741.04	K	Joback Method
tf	276.34	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.40	J/mol×K	519.27	Joback Method
cpg	339.21	J/mol×K	556.23	Joback Method
cpg	356.17	J/mol×K	593.19	Joback Method
cpg	372.28	J/mol×K	630.16	Joback Method
cpg	387.53	J/mol×K	667.12	Joback Method
cpg	401.93	J/mol×K	704.08	Joback Method
cpg	415.47	J/mol×K	741.04	Joback Method
hvapt	56.90	kJ/mol	435.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C499741&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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