trans-Carveyl acetate

Other names:	Carvyl acetate E
	5-Isopropenyl-2-methyl-2-cyclohexen-1-yl acetate-, trans-
	(E)-Carvyl acetate
	t-Carvyl acetate
	trans-Carvyl acetate
Inchi:	InChI=1S/C12H18O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h5,11-12H,1,6-7H2,2-4H3/t1
InchiKey:	YTHRBOFHFYZBRJ-NEPJUHHUSA-N
Formula:	C12H18O2
SMILES:	C=C(C)C1CC=C(C)C(OC(C)=O)C1
Mol. weight [g/mol]:	194.27
CAS:	1134-95-8

Physical Properties

Property code	Value	Unit	Source
gf	-67.40	kJ/mol	Joback Method
hf	-339.88	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.850		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1345.00		NIST Webbook

rinpol	1337.00	NIST Webbook
rinpol	1364.00	NIST Webbook
rinpol	1342.00	NIST Webbook
rinpol	1337.00	NIST Webbook
rinpol	1314.00	NIST Webbook
rinpol	1332.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1331.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1338.00	NIST Webbook
rinpol	1337.00	NIST Webbook
rinpol	1316.00	NIST Webbook
rinpol	1327.00	NIST Webbook
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rinpol	1333.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1337.00	NIST Webbook
rinpol	1307.00	NIST Webbook
rinpol	1337.00	NIST Webbook
rinpol	1327.00	NIST Webbook
rinpol	1327.00	NIST Webbook
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rinpol	1322.00	NIST Webbook
ripol	1759.00	NIST Webbook
ripol	1746.00	NIST Webbook
ripol	1705.00	NIST Webbook
ripol	1732.00	NIST Webbook
ripol	1749.00	NIST Webbook
ripol	1749.00	NIST Webbook
ripol	1747.00	NIST Webbook
ripol	1759.00	NIST Webbook
ripol	1746.00	NIST Webbook
ripol	1759.00	NIST Webbook

ripol	1747.00		NIST Webbook
tb	565.83	K	Joback Method
tc	775.66	K	Joback Method
tf	297.86	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.61	J/mol×K	565.83	Joback Method
cpg	433.54	J/mol×K	600.80	Joback Method
cpg	450.52	J/mol×K	635.77	Joback Method
cpg	466.58	J/mol×K	670.74	Joback Method
cpg	481.72	J/mol×K	705.71	Joback Method
cpg	495.96	J/mol×K	740.68	Joback Method
cpg	509.31	J/mol×K	775.66	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=C1134958&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