Carvyl propionate, cis-

Other names: 5-Isopropenyl-2-methyl-2-cyclohexen-1-yl propionate, cis
cis-Carvyl propionate
Inchi: InChI=1S/C13H20O2/c1-5-13(14)15-12-8-11(9(2)3)7-6-10(12)4/h6,11-12H,2,5,7-8H2,1,3
InchiKey: DFVXNZOMAOGTBL-VXGBXAGGSA-N
Formula: C13H20O2
SMILES: C=C(C)C1CC=C(C)C(OC(=O)CC)C1
Mol. weight [g/mol]: 208.30
CAS: 145032-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-58.98	kJ/mol	Joback Method
hf	-360.52	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	54.17	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.241		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
tb	588.71	K	Joback Method
tc	795.23	K	Joback Method
tf	309.13	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.04	J/mol×K	588.71	Joback Method
cpg	484.54	J/mol×K	623.13	Joback Method
cpg	502.05	J/mol×K	657.55	Joback Method
cpg	518.61	J/mol×K	691.97	Joback Method
cpg	534.21	J/mol×K	726.39	Joback Method
cpg	548.87	J/mol×K	760.81	Joback Method
cpg	562.62	J/mol×K	795.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C145032504&Units=SI

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