Carvacrol, ethyl ether

Inchi: InChI=1S/C12H18O/c1-5-13-12-8-11(9(2)3)7-6-10(12)4/h6-9H,5H2,1-4H3
InchiKey: DOTAGKFIHPPPTK-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCOc1cc(C(C)C)ccc1C
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	35.87	kJ/mol	Joback Method
hf	-214.92	kJ/mol	Joback Method
hfus	17.76	kJ/mol	Joback Method
hvap	47.93	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.517		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	532.58	K	Joback Method
tc	736.76	K	Joback Method
tf	283.69	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.99	J/mol×K	532.58	Joback Method
cpg	389.19	J/mol×K	566.61	Joback Method
cpg	404.62	J/mol×K	600.64	Joback Method
cpg	419.30	J/mol×K	634.67	Joback Method
cpg	433.25	J/mol×K	668.70	Joback Method
cpg	446.46	J/mol×K	702.73	Joback Method
cpg	458.96	J/mol×K	736.76	Joback Method
dvisc	0.0019011	Pa×s	283.69	Joback Method

dvisc	0.0009549	Pa×s	325.17	Joback Method
dvisc	0.0005605	Pa×s	366.65	Joback Method
dvisc	0.0003667	Pa×s	408.13	Joback Method
dvisc	0.0002594	Pa×s	449.62	Joback Method
dvisc	0.0001945	Pa×s	491.10	Joback Method
dvisc	0.0001526	Pa×s	532.58	Joback Method

Sources

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=R200063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume