Ethyleugenol

Inchi: InChI=1S/C12H16O2/c1-4-6-10-7-8-11(14-5-2)12(9-10)13-3/h4,7-9H,1,5-6H2,2-3H3
InchiKey: OTMFQLIUPDESAI-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: C=CCc1ccc(OCC)c(OC)c1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	21.15	kJ/mol	Joback Method
hf	-216.43	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	50.06	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.822		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1425.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1425.00		NIST Webbook
tb	552.12	K	Joback Method
tc	754.25	K	Joback Method
tf	319.16	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.98	J/mol×K	552.12	Joback Method
cpg	446.66	J/mol×K	720.56	Joback Method
cpg	434.47	J/mol×K	686.88	Joback Method
cpg	421.61	J/mol×K	653.19	Joback Method
cpg	408.08	J/mol×K	619.50	Joback Method
cpg	393.87	J/mol×K	585.81	Joback Method
cpg	458.18	J/mol×K	754.25	Joback Method

dvisc	0.0001372	Pa×s	552.12	Joback Method
dvisc	0.0001696	Pa×s	513.29	Joback Method
dvisc	0.0002172	Pa×s	474.47	Joback Method
dvisc	0.0002906	Pa×s	435.64	Joback Method
dvisc	0.0004116	Pa×s	396.81	Joback Method
dvisc	0.0006289	Pa×s	357.99	Joback Method
dvisc	0.0010650	Pa×s	319.16	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=R251922&Units=SI

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