Dihydro-eugenol acetate

Other names: Phenol, 2-methoxy-4-propyl, acetate
Inchi: InChI=1S/C12H16O3/c1-4-5-10-6-7-11(15-9(2)13)12(8-10)14-3/h6-8H,4-5H2,1-3H3
InchiKey: IXIJPFDYLOLJQN-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: CCCc1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]: 208.25
CAS: 33943-26-9

Physical Properties

Property code	Value	Unit	Source
gf	-195.61	kJ/mol	Joback Method
hf	-454.44	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.573		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1536.00		NIST Webbook
tb	609.31	K	Joback Method
tc	815.15	K	Joback Method
tf	370.85	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.81	J/mol×K	609.31	Joback Method
cpg	483.69	J/mol×K	780.85	Joback Method
cpg	472.17	J/mol×K	746.54	Joback Method
cpg	459.92	J/mol×K	712.23	Joback Method
cpg	446.94	J/mol×K	677.92	Joback Method
cpg	433.24	J/mol×K	643.62	Joback Method
cpg	494.48	J/mol×K	815.15	Joback Method

dvisc	0.0001427	Pa×s	609.31	Joback Method
dvisc	0.0001766	Pa×s	569.57	Joback Method
dvisc	0.0002256	Pa×s	529.82	Joback Method
dvisc	0.0003000	Pa×s	490.08	Joback Method
dvisc	0.0004195	Pa×s	450.34	Joback Method
dvisc	0.0006260	Pa×s	410.59	Joback Method
dvisc	0.0010176	Pa×s	370.85	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=C33943269&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