Acetyl eugenol

Other names: Eugenyl acetate
Inchi: InChI=1S/C12H14O3/c1-4-5-10-6-7-11(15-9(2)13)8-12(10)14-3/h4,6-8H,1,5H2,2-3H3
InchiKey: MUFKFMXVLWHCHY-UHFFFAOYSA-N
Formula: C12H14O3
SMILES: C=CCc1ccc(OC(C)=O)cc1OC
Mol. weight [g/mol]: 206.24

Physical Properties

Property code	Value	Unit	Source
gf	-107.77	kJ/mol	Joback Method
hf	-329.01	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.349		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	605.99	K	Joback Method
tc	815.85	K	Joback Method
tf	369.09	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.71	J/mol×K	605.99	Joback Method
cpg	411.50	J/mol×K	640.97	Joback Method
cpg	424.56	J/mol×K	675.94	Joback Method
cpg	436.90	J/mol×K	710.92	Joback Method
cpg	448.51	J/mol×K	745.90	Joback Method
cpg	459.40	J/mol×K	780.88	Joback Method
cpg	469.57	J/mol×K	815.85	Joback Method
dvisc	0.0009921	Pa×s	369.09	Joback Method

dvisc	0.0006199	Pa×s	408.57	Joback Method
dvisc	0.0004207	Pa×s	448.06	Joback Method
dvisc	0.0003041	Pa×s	487.54	Joback Method
dvisc	0.0002307	Pa×s	527.02	Joback Method
dvisc	0.0001819	Pa×s	566.51	Joback Method
dvisc	0.0001480	Pa×s	605.99	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=U284911&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