p-ethyl-«alpha»,«alpha»-dimethyl hydrocinnamic aldehyde

Inchi: InChI=1S/C13H18O/c1-4-11-5-7-12(8-6-11)9-13(2,3)10-14/h5-8,10H,4,9H2,1-3H3
InchiKey: JFTSYAALCNQOKO-UHFFFAOYSA-N
Formula: C13H18O
SMILES: CCc1ccc(CC(C)(C)C=O)cc1
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	64.68	kJ/mol	Joback Method
hf	-180.92	kJ/mol	Joback Method
hfus	17.95	kJ/mol	Joback Method
hvap	52.89	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.017		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1456.80		NIST Webbook
rinpol	1456.80		NIST Webbook
tb	573.93	K	Joback Method
tc	787.33	K	Joback Method
tf	319.63	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.39	J/mol×K	573.93	Joback Method
cpg	492.85	J/mol×K	751.77	Joback Method
cpg	480.26	J/mol×K	716.20	Joback Method
cpg	466.78	J/mol×K	680.63	Joback Method
cpg	452.34	J/mol×K	645.06	Joback Method
cpg	436.90	J/mol×K	609.50	Joback Method
cpg	504.61	J/mol×K	787.33	Joback Method
dvisc	0.0002032	Pa×s	573.93	Joback Method

dvisc	0.0002665	Pa×s	531.55	Joback Method
dvisc	0.0003662	Pa×s	489.16	Joback Method
dvisc	0.0005345	Pa×s	446.78	Joback Method
dvisc	0.0008444	Pa×s	404.40	Joback Method
dvisc	0.0014850	Pa×s	362.01	Joback Method
dvisc	0.0030332	Pa×s	319.63	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=R185890&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