isoeugenyl acetate 2

Other names: (Z)-Isoeugenol acetate
Inchi: InChI=1S/C12H14O3/c1-4-5-10-6-7-11(15-9(2)13)12(8-10)14-3/h4-8H,1-3H3/b5-4-
InchiKey: IUSBVFZKQJGVEP-PLNGDYQASA-N
Formula: C12H14O3
SMILES: CC=Cc1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]: 206.24
CAS: 97412-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-115.39	kJ/mol	Joback Method
hf	-337.22	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.654		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1581.20		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1581.20		NIST Webbook
tb	613.47	K	Joback Method
tc	827.88	K	Joback Method
tf	365.77	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.09	J/mol×K	613.47	Joback Method
cpg	411.97	J/mol×K	649.20	Joback Method
cpg	425.09	J/mol×K	684.94	Joback Method
cpg	437.45	J/mol×K	720.67	Joback Method

cpg	449.08	J/mol×K	756.41	Joback Method
cpg	459.96	J/mol×K	792.14	Joback Method
cpg	470.13	J/mol×K	827.88	Joback Method
dvisc	0.0009291	Pa×s	365.77	Joback Method
dvisc	0.0005581	Pa×s	407.05	Joback Method
dvisc	0.0003683	Pa×s	448.34	Joback Method
dvisc	0.0002607	Pa×s	489.62	Joback Method
dvisc	0.0001947	Pa×s	530.90	Joback Method
dvisc	0.0001516	Pa×s	572.19	Joback Method
dvisc	0.0001222	Pa×s	613.47	Joback Method

Sources

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=C97412232&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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