

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	1581.20		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1566.00		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/molxK	613.47	Joback Method
cpg	459.96	J/molxK	792.14	Joback Method
cpg	449.08	J/molxK	756.41	Joback Method
cpg	437.45	J/molxK	720.67	Joback Method

cpg	425.09	J/molxK	684.94	Joback Method
cpg	411.97	J/molxK	649.20	Joback Method
cpg	470.13	J/molxK	827.88	Joback Method
dvisc	0.0001222	Paxs	613.47	Joback Method
dvisc	0.0001516	Paxs	572.19	Joback Method
dvisc	0.0001947	Paxs	530.90	Joback Method
dvisc	0.0002607	Paxs	489.62	Joback Method
dvisc	0.0003683	Paxs	448.34	Joback Method
dvisc	0.0005581	Paxs	407.05	Joback Method
dvisc	0.0009291	Paxs	365.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97412232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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