

(E)-Methyl isoeugenol

Other names:	trans-Methylisoeugenol (E)-Methyl eugenol (E)-1,2-Dimethoxy-4-propenylbenzene 4-trans-propenylveratrole
Inchi:	InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h4-8H,1-3H3/b5-4+
InchiKey:	NNWHUJCUHAELCL-SNAWJCMRSA-N
Formula:	C11H14O2
SMILES:	CC=Cc1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	178.23
CAS:	6379-72-2

Physical Properties

Property code	Value	Unit	Source
gf	5.11	kJ/mol	Joback Method
hf	-204.00	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.737		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1465.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1461.80		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1460.00		NIST Webbook

rinpol	1460.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	2178.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2209.00		NIST Webbook
tb	536.72	K	Joback Method
tc	746.85	K	Joback Method
tf	304.57	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.08	J/mol×K	536.72	Joback Method
cpg	347.28	J/mol×K	571.74	Joback Method
cpg	360.80	J/mol×K	606.76	Joback Method
cpg	373.65	J/mol×K	641.78	Joback Method
cpg	385.84	J/mol×K	676.80	Joback Method
cpg	397.38	J/mol×K	711.82	Joback Method
cpg	408.27	J/mol×K	746.85	Joback Method
dvisc	0.0010229	Pa×s	304.57	Joback Method
dvisc	0.0005877	Pa×s	343.26	Joback Method
dvisc	0.0003778	Pa×s	381.95	Joback Method
dvisc	0.0002634	Pa×s	420.64	Joback Method
dvisc	0.0001952	Pa×s	459.34	Joback Method
dvisc	0.0001515	Pa×s	498.03	Joback Method
dvisc	0.0001220	Pa×s	536.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6379722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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