

trans-Isoosmorhizole

Other names:	Benzene, 1-(E)-(1-propenyl)-2,4-dimethoxy
Inchi:	InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)8-11(9)13-3/h4-8H,1-3H3/b5-4+
InchiKey:	SKWTXGMULLCOGN-SNAWJCMRSA-N
Formula:	C11H14O2
SMILES:	CC=Cc1ccc(OC)cc1OC
Mol. weight [g/mol]:	178.23

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
ripol	2212.00		NIST Webbook
ripol	2212.00		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

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=R3180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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