

1,4-Dimethoxy-2-methyl-5-(prop-1-en-2-yl)benzene

Inchi:	InChI=1S/C12H16O2/c1-8(2)10-7-11(13-4)9(3)6-12(10)14-5/h6-7H,1H2,2-5H3
InchiKey:	BKYVJXZONZSTIB-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	<chem>C=C(C)c1cc(OC)c(C)cc1OC</chem>
Mol. weight [g/mol]:	192.25
CAS:	39701-09-2

Physical Properties

Property code	Value	Unit	Source
gf	2.97	kJ/mol	Joback Method
hf	-237.69	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	50.80	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.045		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1443.40		NIST Webbook
tb	556.98	K	Joback Method
tc	763.77	K	Joback Method
tf	317.72	K	Joback Method
vc	0.618	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.70	J/molxK	556.98	Joback Method
cpg	393.55	J/molxK	591.45	Joback Method
cpg	407.74	J/molxK	625.91	Joback Method
cpg	421.27	J/molxK	660.38	Joback Method
cpg	434.14	J/molxK	694.84	Joback Method
cpg	446.36	J/molxK	729.31	Joback Method
cpg	457.90	J/molxK	763.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C39701092&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/93-999-1/1-4-Dimethoxy-2-methyl-5-prop-1-en-2-yl-benzene.pdf>

Generated by Cheméo on 2024-08-12 10:40:58.25947383 +0000 UTC m=+2149127.506579176.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.