Benzene, 1,2,3,4-tetramethoxy-5-(2-propenyl)-

Other names:	Benzene, 1-allyl-2,3,4,5-tetramethoxy-
	Allyltetramethoxybenzene
	1-Allyl-2,3,4,5-tetramethoxybenzene
	2,3,4,5-Tetramethoxyallylbenzene
	Benzene, 1-(2-propenyl)-2,3,4,5-tetramethoxy
	l,2,3,4-Tetramethoxy-5-(2)-propenylbenzene
Inchi:	InChI=1S/C13H18O4/c1-6-7-9-8-10(14-2)12(16-4)13(17-5)11(9)15-3/h6,8H,1,7H2,2-5H3
InchiKey:	HRAXJWRHSUTMCS-UHFFFAOYSA-N
Formula:	C13H18O4
SMILES:	C=CCc1cc(OC)c(OC)c(OC)c1OC
Mol. weight [g/mol]:	238.28
CAS:	15361-99-6

Physical Properties

Property code	Value	Unit	Source
gf	-199.69	kJ/mol	Joback Method
hf	-524.45	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.449		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1603.30		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1591.00		NIST Webbook
ripol	2265.00		NIST Webbook
tb	629.80	K	Joback Method
tc	827.53	K	Joback Method
tf	399.93	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.10	J/mol×K	629.80	Joback Method
cpg	493.94	J/mol×K	662.75	Joback Method
cpg	508.16	J/mol×K	695.71	Joback Method
cpg	521.73	J/mol×K	728.66	Joback Method
cpg	534.61	J/mol×K	761.62	Joback Method
cpg	546.77	J/mol×K	794.57	Joback Method
cpg	558.20	J/mol×K	827.53	Joback Method
dvisc	0.0004079	Pa×s	399.93	Joback Method
dvisc	0.0002760	Pa×s	438.24	Joback Method
dvisc	0.0001989	Pa×s	476.55	Joback Method
dvisc	0.0001505	Pa×s	514.87	Joback Method
dvisc	0.0001184	Pa×s	553.18	Joback Method
dvisc	0.0000960	Pa×s	591.49	Joback Method
dvisc	0.0000799	Pa×s	629.80	Joback Method

Sources

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=C15361996&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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