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

Inchi: InChI=1S/C13H18O4/c1-6-7-9-8-10(14-2)12(16-4)13(17-5)11(9)15-3/h6-8H,1-5H3/b7-6+
InchiKey: UZGCZTNAMZBYID-VOTSOKGWSA-N
Formula: C13H18O4
SMILES: CC=Cc1cc(OC)c(OC)c(OC)c1OC
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-207.31	kJ/mol	Joback Method
hf	-532.66	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	59.05	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.754		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1570.00		NIST Webbook
tb	637.28	K	Joback Method
tc	839.03	K	Joback Method
tf	396.61	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.87	J/mol×K	637.28	Joback Method
cpg	494.83	J/mol×K	670.91	Joback Method
cpg	509.13	J/mol×K	704.53	Joback Method
cpg	522.74	J/mol×K	738.16	Joback Method
cpg	535.65	J/mol×K	771.78	Joback Method
cpg	547.83	J/mol×K	805.41	Joback Method
cpg	559.25	J/mol×K	839.03	Joback Method
dvisc	0.0003761	Pa×s	396.61	Joback Method
dvisc	0.0002463	Pa×s	436.72	Joback Method

dvisc	0.0001732	Pa×s	476.83	Joback Method
dvisc	0.0001287	Pa×s	516.94	Joback Method
dvisc	0.0000997	Pa×s	557.06	Joback Method
dvisc	0.0000800	Pa×s	597.17	Joback Method
dvisc	0.0000660	Pa×s	637.28	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=R404998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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