(E)-1-(2',4',5'-Trimethoxyphenyl)butadiene

Inchi: InChI=1S/C13H16O3/c1-5-6-7-10-8-11(14-2)13(16-4)12(9-10)15-3/h5-9H,1H2,2-4H3/b7-
InchiKey: UAJSTXIBAXZQQK-VOTSOKGWSA-N
Formula: C13H16O3
SMILES: C=CC=Cc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-4.84	kJ/mol	Joback Method
hf	-263.54	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.912		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	1708.00		NIST Webbook
tb	606.56	K	Joback Method
tc	813.14	K	Joback Method
tf	360.10	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.86	J/mol×K	606.56	Joback Method
cpg	447.58	J/mol×K	640.99	Joback Method
cpg	461.59	J/mol×K	675.42	Joback Method
cpg	474.89	J/mol×K	709.85	Joback Method
cpg	487.49	J/mol×K	744.28	Joback Method
cpg	499.37	J/mol×K	778.71	Joback Method
cpg	510.55	J/mol×K	813.14	Joback Method
dvisc	0.0005839	Pa×s	360.10	Joback Method
dvisc	0.0003609	Pa×s	401.18	Joback Method

dvisc	0.0002440	Pa×s	442.25	Joback Method
dvisc	0.0001763	Pa×s	483.33	Joback Method
dvisc	0.0001340	Pa×s	524.41	Joback Method
dvisc	0.0001060	Pa×s	565.48	Joback Method
dvisc	0.0000866	Pa×s	606.56	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=R519263&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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