(Z)-1-(3',4'-Dimethoxyphenyl)butadiene

Inchi: InChI=1S/C12H14O2/c1-4-5-6-10-7-8-11(13-2)12(9-10)14-3/h4-9H,1H2,2-3H3/b6-5-
InchiKey: JFHQUUYHTBVHHK-WAYWQWQTSA-N
Formula: C12H14O2
SMILES: C=CC=Cc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	101.37	kJ/mol	Joback Method
hf	-99.21	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.903		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
tb	556.28	K	Joback Method
tc	767.41	K	Joback Method
tf	314.08	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.03	J/mol×K	556.28	Joback Method
cpg	374.45	J/mol×K	591.47	Joback Method
cpg	388.12	J/mol×K	626.66	Joback Method
cpg	401.07	J/mol×K	661.85	Joback Method
cpg	413.31	J/mol×K	697.04	Joback Method
cpg	424.86	J/mol×K	732.23	Joback Method
cpg	435.73	J/mol×K	767.41	Joback Method
dvisc	0.0009698	Pa×s	314.08	Joback Method

dvisc	0.0005576	Pa×s	354.45	Joback Method
dvisc	0.0003590	Pa×s	394.81	Joback Method
dvisc	0.0002508	Pa×s	435.18	Joback Method
dvisc	0.0001862	Pa×s	475.55	Joback Method
dvisc	0.0001448	Pa×s	515.91	Joback Method
dvisc	0.0001169	Pa×s	556.28	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=R519307&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