Benzene, 1,2-dimethoxy-4-(2-nitro-1-propenyl)-

Other names: Benzene, 1,2-dimethoxy-4-(2-nitropropenyl)-
1,2-Dimethoxy-4-(2-nitropropenyl)benzene
1-(3,4-dimethoxyphenyl)-2-nitropropene
Inchi: InChI=1S/C11H13NO4/c1-8(12(13)14)6-9-4-5-10(15-2)11(7-9)16-3/h4-7H,1-3H3/b8-6-
InchiKey: JGFBGRHDJMANRR-VURMDHGXSA-N
Formula: C11H13NO4
SMILES: COc1ccc(C=C(C)[N+](=O)[O-])cc1OC
Mol. weight [g/mol]: 223.23
CAS: 122-47-4

Physical Properties

Property code	Value	Unit	Source
gf	32.11	kJ/mol	Joback Method
hf	-224.55	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	65.13	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.341		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	688.44	K	Joback Method
tc	925.98	K	Joback Method
tf	434.22	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.68	J/mol×K	688.44	Joback Method
cpg	446.12	J/mol×K	728.03	Joback Method
cpg	458.64	J/mol×K	767.62	Joback Method
cpg	470.26	J/mol×K	807.21	Joback Method
cpg	481.00	J/mol×K	846.80	Joback Method
cpg	490.87	J/mol×K	886.39	Joback Method

cpg	499.90	J/mol×K	925.98	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=C122474&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume