

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

Other names:	Benzene, 1,4-dimethoxy-2-(2-nitropropenyl)- 1-(2,5-Dimethoxyphenyl)-2-nitropropene 2,5-Dimethoxy-«beta»-methyl-«beta»-nitrostyrene 1,4-dimethoxy-2-(2-nitropropenyl)benzene
Inchi:	InChI=1S/C11H13NO4/c1-8(12(13)14)6-9-7-10(15-2)4-5-11(9)16-3/h4-7H,1-3H3/b8-6+
InchiKey:	MQFREHNTGKNSRH-SOFGYWHQSA-N
Formula:	C11H13NO4
SMILES:	COc1ccc(OC)c(C=C(C)[N+](=O)[O-])c1
Mol. weight [g/mol]:	223.23
CAS:	18790-57-3

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/molxK	688.44	Joback Method
cpg	446.12	J/molxK	728.03	Joback Method
cpg	458.64	J/molxK	767.62	Joback Method
cpg	470.26	J/molxK	807.21	Joback Method
cpg	481.00	J/molxK	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=C18790573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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