Benzene, 1-methoxy-2-(2-nitroethenyl)-

Other names:	1-Methoxy-2-(2-nitroethenyl)benzene
	1-(2-Methoxyphenyl)-2-nitroethene
	2-(2-Nitrovinyl)anisole
	2-Methoxy-«beta»-nitrostyrene
	o-Methoxy-«beta»-nitrostyrene
	Anisole, o-(2-nitrovinyl)-
	1-Methoxy-2-(2-nitrovinyl)benzene
	Ethene,-1-(2-methoxyphenyl)-2-nitro-
	NSC 170699
	NSC 59450
Inchi:	InChI=1S/C9H9NO3/c1-13-9-5-3-2-4-8(9)6-7-10(11)12/h2-7H,1H3/b7-6+
InchiKey:	FVKSRNVYJXQCLK-VOTSOKGWSA-N
Formula:	C9H9NO3
SMILES:	COc1ccccc1C=C[N+](=O)[O-]
Mol. weight [g/mol]:	179.17
CAS:	3316-24-3

Physical Properties

Property code	Value	Unit	Source
gf	138.45	kJ/mol	Joback Method
hf	-29.79	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	1.943		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	615.40	K	Joback Method
tc	861.96	K	Joback Method
tf	390.89	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.97	J/mol×K	615.40	Joback Method
cpg	325.17	J/mol×K	656.49	Joback Method
cpg	336.46	J/mol×K	697.59	Joback Method
cpg	346.90	J/mol×K	738.68	Joback Method
cpg	356.53	J/mol×K	779.77	Joback Method
cpg	365.40	J/mol×K	820.86	Joback Method
cpg	373.54	J/mol×K	861.96	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=C3316243&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