3,4-Methylenedioxy-«beta»-nitrostyrene

Other names:	Styrene, 3,4-methylenedioxy-«beta»-nitro- 1,3-Benzodioxole, 5-(2-nitroethenyl)- 1,3-Benzodioxole, 5-nitrovinyl- 1-(2-Nitrovinyl)-3,4-methylenedioxybenzene 3,4-(Methylenedioxy)-beta-nitrostyrene 3,4-Methylenedioxy-1-(2-nitrovinyl)benzene 5-(2-Nitrovinyl)-1,3-benzodioxole Styrene, 3,4-(methylenedioxy)-b-nitro- Ethene, 1-(3,4-methylendioxyphenyl)-2-nitro- Benzene, 2-nitroethenyl, 3,4-methylenedioxy NSC 10120 NSC 105303 NSC 170724
Inchi:	InChI=1S/C9H7NO4/c11-10(12)4-3-7-1-2-8-9(5-7)14-6-13-8/h1-5H,6H2/b4-3+
InchiKey:	KFLWBZPSJQPRDD-ONEGZZNKSA-N
Formula:	C9H7NO4
SMILES:	O=[N+]([O-])C=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	193.16
CAS:	1485-00-3

Physical Properties

Property code	Value	Unit	Source
gf	130.04	kJ/mol	Joback Method
hf	-79.90	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	65.02	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	1.663		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	663.27	K	Joback Method
tc	925.05	K	Joback Method
tf	456.50	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.98	J/mol×K	663.27	Joback Method
cpg	333.59	J/mol×K	706.90	Joback Method
cpg	343.26	J/mol×K	750.53	Joback Method
cpg	352.13	J/mol×K	794.16	Joback Method
cpg	360.32	J/mol×K	837.79	Joback Method
cpg	367.94	J/mol×K	881.42	Joback Method
cpg	375.13	J/mol×K	925.05	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=C1485003&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