Benzene, (2-nitropropen-1-yl)-

Other names:	Benzene, (2-nitro-1-propenyl)-
	«beta»-Methyl-«beta»-nitrostyrene
	1-Phenyl-2-nitro-1-propene
	(2-Nitropropenyl)benzene
	1-Phenyl-2-nitropropene
	2-Nitro-1-phenyl-1-propene
	(2-Nitro-1-propenyl)benzene
	1-(2-Nitropropenyl)benzene
	1-Phenyl-2-nitro-propylen-(1,2)
	Benzene, (2-nitropropenyl)-
	Phenyl-2-nitropropene -
	1-Phenyl-2-nitro-2-methylethene
	2-Nitro-3-phenyl-2-propene
	NSC 2014
Inchi:	InChI=1S/C9H9NO2/c1-8(10(11)12)7-9-5-3-2-4-6-9/h2-7H,1H3/b8-7+
InchiKey:	WGSVFWFSJDAYBM-BQYQJAHWSA-N
Formula:	C9H9NO2
SMILES:	CC(=Cc1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]:	163.17
CAS:	705-60-2

Physical Properties

Property code	Value	Unit	Source
chs	-4812.40 ± 2.10	kJ/mol	NIST Webbook
gf	244.53	kJ/mol	Joback Method
hf	104.11	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.324		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	587.88	K	Joback Method
tc	842.33	K	Joback Method
tf	342.18	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.10	J/mol×K	587.88	Joback Method
cpg	304.05	J/mol×K	630.29	Joback Method
cpg	315.91	J/mol×K	672.70	Joback Method
cpg	326.78	J/mol×K	715.11	Joback Method
cpg	336.74	J/mol×K	757.51	Joback Method
cpg	345.87	J/mol×K	799.92	Joback Method
cpg	354.27	J/mol×K	842.33	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=C705602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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