

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

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:	C/C(=C\c1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]:	163.18

Physical Properties

Property code	Value	Unit	Source
chs	-4812.40 ± 2.10	kJ/mol	NIST Webbook
hf	96.32	kJ/mol	Cheméo Relay (1.0)
hfus	23.36	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
logp	2.324		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
tb	541.83	K	Cheméo Relay (1.0)
tf	353.07	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C705602&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/40-783-8/Benzene-2-nitro-1-propenyl.pdf>

Generated by Cheméo on 2026-07-22 00:12:36.955982797 +0000 UTC m=+190252.797868174.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.