

Benzene, 1-ethenyl-3-nitro-

Other names:	3-Nitrostyrene m-Nitrostyrene Styrene, m-nitro- m-Vinylnitrobenzene
Inchi:	InChI=1S/C8H7NO2/c1-2-7-4-3-5-8(6-7)9(10)11/h2-6H,1H2
InchiKey:	SYZVQXIUVGKCBJ-UHFFFAOYSA-N
Formula:	C8H7NO2
SMILES:	<chem>C=Cc1cccc([N+](=O)[O-])c1</chem>
Mol. weight [g/mol]:	149.15
CAS:	586-39-0

Physical Properties

Property code	Value	Unit	Source
gf	242.65	kJ/mol	Joback Method
hf	131.28	kJ/mol	Joback Method
hfus	20.21	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.238		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	562.62	K	Joback Method
tc	812.97	K	Joback Method
tf	360.71	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.77	J/molxK	562.62	Joback Method
cpg	257.15	J/molxK	604.34	Joback Method
cpg	267.64	J/molxK	646.07	Joback Method
cpg	277.29	J/molxK	687.79	Joback Method
cpg	286.15	J/molxK	729.52	Joback Method

cpg	294.28	J/mol×K	771.24	Joback Method
cpg	301.74	J/mol×K	812.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C586390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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