Benzene, 1-ethynyl-4-nitro-

Other names: 4-Nitrophenylacetylene
1-Ethynyl-4-nitrobenzene
Inchi: InChI=1S/C8H5NO2/c1-2-7-3-5-8(6-4-7)9(10)11/h1,3-6H
InchiKey: GAZZTEJDUGESGQ-UHFFFAOYSA-N
Formula: C8H5NO2
SMILES: C#Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 147.13
CAS: 937-31-5

Physical Properties

Property code	Value	Unit	Source
gf	377.88	kJ/mol	Joback Method
hf	297.75	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	52.79	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.576		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
tb	556.06	K	Joback Method
tc	820.27	K	Joback Method
tf	409.44	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.08	J/mol×K	556.06	Joback Method
cpg	238.38	J/mol×K	600.09	Joback Method
cpg	247.79	J/mol×K	644.13	Joback Method
cpg	256.38	J/mol×K	688.16	Joback Method
cpg	264.20	J/mol×K	732.20	Joback Method
cpg	271.33	J/mol×K	776.23	Joback Method
cpg	277.82	J/mol×K	820.27	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=C937315&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