Benzonitrile, 4-nitro-

Other names:	4-cyano-1-nitrobenzene
	4-cyanonitrobenzene
	4-nitrobenzenenitrile
	4-nitrobenzonitrile
	benzonitrile, p-nitro-
	p-cyanonitrobenzene
	p-nitrobenzonitrile
Inchi:	InChI=1S/C7H4N2O2/c8-5-6-1-3-7(4-2-6)9(10)11/h1-4H
InchiKey:	NKJIFDNZPGLLSH-UHFFFAOYSA-N
Formula:	C7H4N2O2
SMILES:	N#Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	148.12
CAS:	619-72-7

Physical Properties

Property code	Value	Unit	Source
affp	775.70	kJ/mol	NIST Webbook
basg	745.10	kJ/mol	NIST Webbook
ea	1.77 ± 0.05	eV	NIST Webbook
ea	1.69 ± 0.09	eV	NIST Webbook
ea	1.73 ± 0.10	eV	NIST Webbook
gf	279.57	kJ/mol	Joback Method
hf	191.37	kJ/mol	Joback Method
hfus	20.41	kJ/mol	Joback Method
hsub	91.10 ± 1.30	kJ/mol	NIST Webbook
hvap	61.18	kJ/mol	Joback Method
ie	10.20 ± 0.10	eV	NIST Webbook
ie	10.59 ± 0.05	eV	NIST Webbook
log10ws	-2.47		Crippen Method
logp	1.466		Crippen Method
mcvol	104.530	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	645.14	K	Joback Method
tc	909.48	K	Joback Method
tf	416.19	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.38	J/mol×K	645.14	Joback Method
cpg	241.66	J/mol×K	689.20	Joback Method
cpg	249.20	J/mol×K	733.25	Joback Method
cpg	256.04	J/mol×K	777.31	Joback Method
cpg	262.24	J/mol×K	821.36	Joback Method
cpg	267.83	J/mol×K	865.42	Joback Method
cpg	272.86	J/mol×K	909.48	Joback Method
hfust	17.73	kJ/mol	420.60	NIST Webbook
hsubt	90.50 ± 1.30	kJ/mol	313.50	NIST Webbook

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=C619727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility Determination and Modeling for 4-Nitrobenzonitrile in Binary Solvent Mixtures of Ethyl Acetate Plus (Methanol, Ethanol, n-Propanol, and Isopropanol):	https://www.doi.org/10.1021/acs.jced.8b00555

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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