Benzonitrile, 2-nitro-

Other names:	Benzonitrile, o-nitro-
	o-Cyanonitrobenzene
	o-Nitrobenzonitrile
	2-Nitrobenzonitrile
	2-Nitrobenzoic acid nitrile
Inchi:	InChI=1S/C7H4N2O2/c8-5-6-3-1-2-4-7(6)9(10)11/h1-4H
InchiKey:	SWBDKCMOLSUXRH-UHFFFAOYSA-N
Formula:	C7H4N2O2
SMILES:	N#Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	148.12
CAS:	612-24-8

Physical Properties

Property code	Value	Unit	Source
ea	1.98 ± 0.05	eV	NIST Webbook
ea	1.61 ± 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	88.10 ± 1.40	kJ/mol	NIST Webbook
hvap	61.18	kJ/mol	Joback Method
ie	10.52 ± 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	262.24	J/mol×K	821.36	Joback Method
cpg	267.83	J/mol×K	865.42	Joback Method
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	272.86	J/mol×K	909.48	Joback Method
hfust	15.72	kJ/mol	382.70	NIST Webbook
hsubt	87.90 ± 1.40	kJ/mol	304.00	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=C612248&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
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