Benzene, 1-isocyano-4-nitro-

Other names: Phenyl isocyanide, p-nitro-
p-Nitrophenyl isocyanide
Inchi: InChI=1S/C7H4N2O2/c1-8-6-2-4-7(5-3-6)9(10)11/h2-5H
InchiKey: WQFPYEBGLBCQOY-UHFFFAOYSA-N
Formula: C7H4N2O2
SMILES: [C-]#[N+]c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 148.12
CAS: 1984-23-2

Physical Properties

Property code	Value	Unit	Source
gf	279.57	kJ/mol	Joback Method
hf	191.37	kJ/mol	Joback Method
hfus	20.41	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	2.146		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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1984232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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