

4-NITROPHENYLACETONITRILE

Other names:	(p-Nitrobenzene)acetonitrile (p-Nitrophenyl)acetonitrile 2-(4-nitrophenyl)acetonitrile 4-Nitrobenzeneacetonitrile 4-Nitrobenzyl cyanide 4-Nitrobenzyl nitrile Acetonitrile, (p-nitrophenyl)- NSC 5396 p-Nitro-«alpha»-tolunitrile p-Nitrobenzyl cyanide p-nitrophenylacetonitrile
Inchi:	InChI=1S/C8H6N2O2/c9-6-5-7-1-3-8(4-2-7)10(11)12/h1-4H,5H2
InchiKey:	PXNJGLAVKOXITN-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	N#CCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	162.15

Physical Properties

Property code	Value	Unit	Source
hf	195.10	kJ/mol	Cheméo Relay (1.0)
hfus	23.00	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Cheméo Relay (1.0)
ie	10.11 ± 0.04	eV	NIST Webbook
log10ws	-2.75		Cheméo Relay (1.0)
logp	1.661		Crippen Method
mcvol	118.620	ml/mol	McGowan Method
tb	570.03	K	Cheméo Relay (1.0)
tf	392.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.60	J/mol×K	668.02	Joback Method
cpg	288.90	J/mol×K	711.02	Joback Method

cpg	297.41	J/mol×K	754.02	Joback Method
cpg	305.17	J/mol×K	797.02	Joback Method
cpg	312.24	J/mol×K	840.02	Joback Method
cpg	318.66	J/mol×K	883.02	Joback Method
cpg	324.47	J/mol×K	926.02	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C555215&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

4-Nitrophenylcyanide Solubility in Several Nonaqueous Solvent Mixtures: Determination and Modeling: <https://www.doi.org/10.1021/acs.jced.9b00005>

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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