

Benzaldehyde, 4-nitro-

Other names:	4-nitrobenzaldehyde Benzaldehyde, p-nitro- p-Formylnitrobenzene p-nitrobenzaldehyde
Inchi:	InChI=1S/C7H5NO3/c9-5-6-1-3-7(4-2-6)8(10)11/h1-5H
InchiKey:	BXRFQSNOROATLV-UHFFFAOYSA-N
Formula:	C7H5NO3
SMILES:	O=Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	151.12
CAS:	555-16-8

Physical Properties

Property code	Value	Unit	Source
affp	795.10	kJ/mol	NIST Webbook
basg	763.20	kJ/mol	NIST Webbook
chs	-3318.00	kJ/mol	NIST Webbook
chs	-3316.49	kJ/mol	NIST Webbook
ea	1.64 ± 0.09	eV	NIST Webbook
ea	1.65 ± 0.09	eV	NIST Webbook
ea	1.69 ± 0.09	eV	NIST Webbook
gf	46.87	kJ/mol	Joback Method
hf	-59.09	kJ/mol	Joback Method
hfs	-152.70	kJ/mol	NIST Webbook
hfs	-151.00	kJ/mol	NIST Webbook
hfus	21.19	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
ie	10.37	eV	NIST Webbook
ie	10.27 ± 0.01	eV	NIST Webbook
ie	10.27 ± 0.01	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	1.407		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
rinpol	1291.80		NIST Webbook
rinpol	1302.20		NIST Webbook
tb	591.72	K	Joback Method
tc	843.45	K	Joback Method

tf	380.35	K	Thermodynamic modelling for solubility of 4-nitrobenzaldehyde in different solvents at temperature range from (273.15 to 313.15) K and mixing properties of solutions
tf	375.15 ± 2.50	K	NIST Webbook
tf	377.15 ± 2.00	K	NIST Webbook
tf	380.00 ± 2.00	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.64	J/mol×K	591.72	Joback Method
cpg	242.09	J/mol×K	633.68	Joback Method
cpg	250.75	J/mol×K	675.63	Joback Method
cpg	258.68	J/mol×K	717.59	Joback Method
cpg	265.91	J/mol×K	759.54	Joback Method
cpg	272.49	J/mol×K	801.50	Joback Method
cpg	278.45	J/mol×K	843.45	Joback Method

Sources

Thermodynamic modelling for solubility of 4-nitrobenzaldehyde in different solvents at the temperature range from (273.15 to 313.15) K and mixing properties of solutions.

McGowan Method:

NIST Webbook:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.jct.2016.09.012>

<https://www.doi.org/10.1021/acs.jced.8b01067>

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C555168&Units=SI>

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

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

Legend

afp: Proton affinity

basg: Gas basicity

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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