Benzaldehyde, 3-nitro-

Other names:	3-Formylnitrobenzene
	3-nitrobenzaldehyde
	5-Nitrobenzaldehyde
	Benzaldehyde, m-nitro-
	m-nitrobenzaldehyde
Inchi:	InChI=1S/C7H5NO3/c9-5-6-2-1-3-7(4-6)8(10)11/h1-5H
InchiKey:	ZETIVVHRRQLWFW-UHFFFAOYSA-N
Formula:	C7H5NO3
SMILES:	O=Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	151.12
CAS:	99-61-6

Physical Properties

Property code	Value	Unit	Source
chs	-3350.00	kJ/mol	NIST Webbook
ea	1.34 ± 0.09	eV	NIST Webbook
ea	1.43 ± 0.10	eV	NIST Webbook
gf	46.87	kJ/mol	Joback Method
hf	-59.09	kJ/mol	Joback Method
hfs	-120.00	kJ/mol	NIST Webbook
hfus	21.19	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.407		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
rinpol	1314.50		NIST Webbook
rinpol	1304.20		NIST Webbook
tb	591.72	K	Joback Method
tc	843.45	K	Joback Method
tf	328.22	K	Solubility measurement and thermodynamic functions of 3-nitrobenzaldehyde in different solvents at elevated temperatures
tf	331.65 ± 2.00	K	NIST Webbook
tf	330.25 ± 1.00	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.49	J/mol×K	801.50	Joback Method
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	278.45	J/mol×K	843.45	Joback Method
hvapt	62.00	kJ/mol	476.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	3.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99616&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility measurement and thermodynamic functions of 3-nitrobenzaldehyde in different solvents at elevated temperatures:	https://www.doi.org/10.1016/j.jct.2016.10.040
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume