Benzaldehyde, 2-nitro-

Other names: Benzaldehyde, o-nitro-
o-Nitrobenzaldehyde
2-Nitrobenzaldehyde
Inchi: InChI=1S/C7H5NO3/c9-5-6-3-1-2-4-7(6)8(10)11/h1-5H
InchiKey: CMWKITSNTDAEDT-UHFFFAOYSA-N
Formula: C7H5NO3
SMILES: O=Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 151.12
CAS: 552-89-6

Physical Properties

Property code	Value	Unit	Source
chs	-3331.00	kJ/mol	NIST Webbook
ea	1.56 ± 0.10	eV	NIST Webbook
gf	46.87	kJ/mol	Joback Method
hf	-59.09	kJ/mol	Joback Method
hfs	-139.00	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	1277.00		NIST Webbook
rinpol	1271.00		NIST Webbook
tb	591.72	K	Joback Method
tc	843.45	K	Joback Method
tf	312.65 ± 1.50	K	NIST Webbook
tf	316.00 ± 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
hvapt	58.70	kJ/mol	468.50	NIST Webbook
hvapt	59.50	kJ/mol	453.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.20	K	3.10	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C552896&Units=SI

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