

4-Nitrobenzoyl chloride

Other names:	p-Nitrobenzoyl chloride Benzoyl chloride, 4-nitro- p-Nitrobenzoic acid chloride Benzoyl chloride, p-nitro- Nitrobenzoyl chloride, 4- 4-Nitrobenzoic acid chloride
Inchi:	InChI=1S/C7H4ClNO3/c8-7(10)5-1-3-6(4-2-5)9(11)12/h1-4H
InchiKey:	SKDHHIUENRGTHK-UHFFFAOYSA-N
Formula:	C7H4ClNO3
SMILES:	O=C(Cl)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	185.56
CAS:	122-04-3

Physical Properties

Property code	Value	Unit	Source
gf	5.54	kJ/mol	Joback Method
hf	-100.70 ± 7.30	kJ/mol	NIST Webbook
hfs	-199.60 ± 3.60	kJ/mol	NIST Webbook
hfus	24.70	kJ/mol	Joback Method
hsub	98.90 ± 6.30	kJ/mol	NIST Webbook
hvap	61.84	kJ/mol	Joback Method
ie	10.66 ± 0.01	eV	NIST Webbook
log10ws	-3.01		Crippen Method
logp	1.974		Crippen Method
mcvol	116.960	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	634.36	K	Joback Method
tc	895.19	K	Joback Method
tf	344.70 ± 1.00	K	NIST Webbook
vc	0.457	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
---------------	-------	------	-----------------	--------

cpg	250.84	J/mol×K	634.36	Joback Method
cpg	259.60	J/mol×K	677.83	Joback Method
cpg	267.55	J/mol×K	721.30	Joback Method
cpg	274.74	J/mol×K	764.78	Joback Method
cpg	281.22	J/mol×K	808.25	Joback Method
cpg	287.03	J/mol×K	851.72	Joback Method
cpg	292.21	J/mol×K	895.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	476.70	K	14.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/51-302-9/4-Nitrobenzoyl-chloride.pdf>

Generated by Cheméo on 2024-04-23 15:58:24.596117908 +0000 UTC m=+16177153.516695222.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.