

P-NITROBENZOYL CHLORIDE

Other names:	4-Nitrobenzoic acid chloride Benzoyl chloride, 4-nitro- Benzoyl chloride, p-nitro- Nitrobenzoyl chloride, 4- p-Nitrobenzoic acid chloride p-Nitrobenzoyl 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]:	185.57

Physical Properties

Property code	Value	Unit	Source
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	79.92	kJ/mol	Cheméo Relay (1.0)
ie	10.66 ± 0.01	eV	NIST Webbook
log10ws	-3.05		Cheméo Relay (1.0)
logp	1.974		Crippen Method
mcvol	116.960	ml/mol	McGowan Method
tb	532.08	K	Cheméo Relay (1.0)
tf	344.70 ± 1.00	K	NIST Webbook

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C122043&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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