Benzoyl chloride, 3-nitro-

Other names:	3-Nitrobenzoyl chloride
	Benzoyl chloride, m-nitro-
	Chlorid kyseliny m-nitrobenzoove
	m-Nitrobenzoyl chloride
Inchi:	InChI=1S/C7H4ClNO3/c8-7(10)5-2-1-3-6(4-5)9(11)12/h1-4H
InchiKey:	NXTNASSYJUXJDV-UHFFFAOYSA-N
Formula:	C7H4ClNO3
SMILES:	O=C(Cl)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	185.56
CAS:	121-90-4

Physical Properties

Property code	Value	Unit	Source
gf	5.54	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	61.84	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	1.974		Crippen Method
mcvol	116.960	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	549.70	K	NIST Webbook
tc	895.19	K	Joback Method
tf	431.05	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.03	J/mol×K	851.72	Joback Method
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	292.21	J/mol×K	895.19	Joback Method
hvapt	62.40	kJ/mol	489.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.82751e+01
Coeff. B	-7.50643e+03
Temperature range (K), min.	417.31
Temperature range (K), max.	579.04

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C121904&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume