

Carbonochloridic acid, 4-nitrophenyl ester

Other names:	Formic acid, chloro-, p-nitrophenyl ester p-Nitrophenoxycarbonyl chloride p-Nitrophenyl chlorocarbonate p-Nitrophenyl chloroformate Chloroformic acid p-nitrophenyl ester 4-Nitrophenyl chloroformate
Inchi:	InChI=1S/C7H4ClNO4/c8-7(10)13-6-3-1-5(2-4-6)9(11)12/h1-4H
InchiKey:	NXLNNXIXOYSCMB-UHFFFAOYSA-N
Formula:	C7H4ClNO4
SMILES:	O=C(Cl)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	201.56
CAS:	7693-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-99.46	kJ/mol	Joback Method
hf	-234.05	kJ/mol	Joback Method
hfus	25.88	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.332		Crippen Method
mcvol	122.830	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
tb	656.78	K	Joback Method
tc	912.96	K	Joback Method
tf	453.28	K	Joback Method
vc	0.474	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.80	J/mol×K	656.78	Joback Method
cpg	280.50	J/mol×K	699.48	Joback Method
cpg	288.43	J/mol×K	742.17	Joback Method

cpg	295.60	J/mol×K	784.87	Joback Method
cpg	302.04	J/mol×K	827.56	Joback Method
cpg	307.76	J/mol×K	870.26	Joback Method
cpg	312.78	J/mol×K	912.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.70	K	2.50	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7693461&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
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

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