

4-CHLORO-3-NITROBENZOPHENONE

Other names:	Methanone, (4-chloro-3-nitrophenyl)(phenyl) Benzophenone, 4-chloro-3-nitro-
Inchi:	InChI=1S/C13H8ClNO3/c14-11-7-6-10(8-12(11)15(17)18)13(16)9-4-2-1-3-5-9/h1-8H
InchiKey:	YBDBYPQFIMSFJW-UHFFFAOYSA-N
Formula:	C13H8ClNO3
SMILES:	O=C(c1ccccc1)c1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	261.66

Physical Properties

Property code	Value	Unit	Source
hf	-8.17	kJ/mol	Cheméo Relay (1.0)
hfus	33.89	kJ/mol	Joback Method
hvap	98.77	kJ/mol	Cheméo Relay (1.0)
ie	9.72	eV	Cheméo Relay (1.0)
log10ws	-4.43		Cheméo Relay (1.0)
logp	3.479		Crippen Method
mcvol	177.740	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	621.67	K	Cheméo Relay (1.0)
tc	941.93	K	Cheméo Relay (1.0)
tf	349.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.99	J/mol×K	803.30	Joback Method
cpg	462.69	J/mol×K	849.07	Joback Method
cpg	472.25	J/mol×K	894.83	Joback Method
cpg	480.76	J/mol×K	940.60	Joback Method
cpg	488.32	J/mol×K	986.36	Joback Method
cpg	495.02	J/mol×K	1032.13	Joback Method
cpg	500.95	J/mol×K	1077.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	508.20	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56107029&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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

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