

3-Nitrobenzophenone

Other names:	m-Nitrobenzophenone Methanone, (3-nitrophenyl)(phenyl)-
Inchi:	InChI=1S/C13H9NO3/c15-13(10-5-2-1-3-6-10)11-7-4-8-12(9-11)14(16)17/h1-9H
InchiKey:	MFYLRNKOXORIPK-UHFFFAOYSA-N
Formula:	C13H9NO3
SMILES:	O=C(c1ccccc1)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	227.22
CAS:	2243-80-3

Physical Properties

Property code	Value	Unit	Source
ea	1.28 ± 0.09	eV	NIST Webbook
gf	180.40	kJ/mol	Joback Method
hf	26.60	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	73.08	kJ/mol	Joback Method
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	-4.08		Crippen Method
logp	2.826		Crippen Method
mcvol	165.500	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	760.89	K	Joback Method
tc	1033.69	K	Joback Method
tf	495.17	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.87	J/molxK	760.89	Joback Method
cpg	446.05	J/molxK	806.36	Joback Method
cpg	456.98	J/molxK	851.82	Joback Method
cpg	466.76	J/molxK	897.29	Joback Method
cpg	475.50	J/molxK	942.75	Joback Method

cpg	483.29	J/mol×K	988.22	Joback Method
cpg	490.24	J/mol×K	1033.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	507.20	K	2.40	NIST Webbook

Sources

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=C2243803&Units=SI
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
ea:	Electron affinity
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
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

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