

Ethanone, 1-(3-nitrophenyl)-

Other names:	(3-Nitrophenyl) methyl ketone 1-(3-nitrophenyl)ethanone 1-Acetyl-3-nitrobenzene 3'-nitroacetophenone 3-Nitroacetofenon 3-Nitroacetophenone Methyl 3-nitrophenyl ketone NSC 5511 USAF MA-1 acetophenone, 3'-nitro- m-Acetylnitrobenzene m-nitroacetophenone
Inchi:	InChI=1S/C8H7NO3/c1-6(10)7-3-2-4-8(5-7)9(11)12/h2-5H,1H3
InchiKey:	ARKIFHPFTHVKDT-UHFFFAOYSA-N
Formula:	C8H7NO3
SMILES:	CC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	165.15
CAS:	121-89-1

Physical Properties

Property code	Value	Unit	Source
affp	826.00	kJ/mol	NIST Webbook
basg	794.10	kJ/mol	NIST Webbook
ea	1.33 ± 0.10	eV	NIST Webbook
gf	25.89	kJ/mol	Joback Method
hf	-106.73	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	59.68	kJ/mol	Joback Method
ie	9.89 ± 0.05	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	1.797		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	1506.10		NIST Webbook
rinpol	1410.80		NIST Webbook
rinpol	1410.80		NIST Webbook
tb	475.20	K	NIST Webbook

tc	871.76	K	Joback Method
tf	349.68	K	Solubility Measurement and Modeling of 1-(3-nitrophenyl)Ethanone and 1-(4-nitrophenyl)Ethenone in Nine Pure Organic Solvents from T = (278.15 to 318.15) K and Mixing Properties of Solutions
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.23	J/mol×K	619.81	Joback Method
cpg	287.00	J/mol×K	661.80	Joback Method
cpg	296.90	J/mol×K	703.79	Joback Method
cpg	305.97	J/mol×K	745.79	Joback Method
cpg	314.27	J/mol×K	787.78	Joback Method
cpg	321.82	J/mol×K	829.77	Joback Method
cpg	328.68	J/mol×K	871.76	Joback Method
hsubt	110.00	kJ/mol	318.00	NIST Webbook
hvapt	99.10	kJ/mol	298.15	Standard molar enthalpies of formation of 3'- and 4'-nitroacetophenones

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.20	K	2.40	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C121891&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Standard molar enthalpies of formation of 3'- and 4'-nitroacetophenones: <https://www.doi.org/10.1016/j.jct.2011.01.006>
 Research and comparison of solid-liquid phase equilibrium and solubility phase diagrams of 1-(3-nitrophenyl)ethanone and 1-(4-nitrophenyl)ethanone in different Organic Solvents from T = (278.15 to 318.15) K and Mixing Properties of Solutions: <https://www.doi.org/10.1016/j.jct.2019.03.028>
 Solubility Measurement and Modeling of 1-(3-nitrophenyl)ethanone and 1-(4-nitrophenyl)ethanone in Nine Pure Organic Solvents from T = (278.15 to 318.15) K and Mixing Properties of Solutions: <https://www.doi.org/10.1021/acs.jced.8b00192>
 Joback Method: https://en.wikipedia.org/wiki/Joback_method
 Joback Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
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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