

Acetophenone, 4'-nitro-

Other names: 1-(4-Nitrophenyl)ethan-1-one
1-(4-nitrophenyl)ethanone
1-Acetyl-4-nitrobenzene
4'-nitroacetophenone
4-Acetylnitrobenzene
4-Nitroacetophenone
Ethanone, 1-(4-nitrophenyl)-
Methyl 4-nitrophenyl ketone
Methyl-p-nitrophenyl ketone
NSC 41590
PNAP
Paranitroacetophenone
p-Acetylnitrobenzene
p-Nitrophenyl methyl ketone
p-nitroacetophenone

Inchi: InChI=1S/C8H7NO3/c1-6(10)7-2-4-8(5-3-7)9(11)12/h2-5H,1H3

InchiKey: YQYGPGKTNQNXMH-UHFFFAOYSA-N

Formula: C8H7NO3

SMILES: CC(=O)c1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 165.15

CAS: 100-19-6

Physical Properties

Property code	Value	Unit	Source
affp	824.30	kJ/mol	NIST Webbook
basg	792.50	kJ/mol	NIST Webbook
chs	-3933.00	kJ/mol	NIST Webbook
ea	1.54 ± 0.09	eV	NIST Webbook
ea	1.41 ± 0.09	eV	NIST Webbook
ea	1.57 ± 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	10.20 ± 0.10	eV	NIST Webbook
ie	10.07 ± 0.02	eV	NIST Webbook
ie	9.98	eV	NIST Webbook

ie	10.05	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
tb	475.20	K	NIST Webbook
tb	421.70	K	NIST Webbook
tc	871.76	K	Joback Method
tf	354.15	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
tf	353.65 ± 1.50	K	NIST Webbook
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.82	J/mol×K	829.77	Joback Method
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	328.68	J/mol×K	871.76	Joback Method
hvapt	97.00	kJ/mol	298.15	Standard molar enthalpies of formation of 3'- and 4'-nitroacetophenones

Sources

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:
NIST Webbook:

<https://www.doi.org/10.1021/acs.jced.8b00192>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C100196&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 ternary phase diagrams of 1-(3-nitrophenyl)ethanone + 1-(4-nitrophenyl)ethanone in different solvents <https://www.doi.org/10.1016/j.jct.2019.03.028>

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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