Acetamide, N-(4-methylphenyl)-

Other names:	1-acetamido-4-methylbenzene
	4'-methylacetanilide
	4-(Acetylamino)toluene
	4-Acetotoluide
	4-Acetotoluidide
	4-Methylacetanilide
	Acet-p-toluidide
	Acetyl-p-toluidine
	N-(4-methylphenyl)acetamide
	N-Acetyl-p-toluidide
	N-acetyl-4-methylaniline
	N-acetyl-p-toluidine
	NSC 7644
	p-Acetotoluidine
	p-acetamidotoluene
	p-acetotoluide
	p-acetotoluidide
	p-methylacetanilide
Inchi:	InChI=1S/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)
InchiKey:	YICAMJWHIUMFDI-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CC(=O)Nc1ccc(C)cc1
Mol. weight [g/mol]:	149.19
CAS:	103-89-9

Physical Properties

Property code	Value	Unit	Source
chs	-4920.72	kJ/mol	NIST Webbook
gf	88.15	kJ/mol	Joback Method
hf	-63.14	kJ/mol	Joback Method
hfus	29.40	kJ/mol	Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography
hvap	51.75	kJ/mol	Joback Method
ie	7.75 ± 0.02	eV	NIST Webbook
ie	8.20 ± 0.20	eV	NIST Webbook

log10ws	-2.15		Crippen Method
logp	1.953		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	580.20	K	NIST Webbook
tc	761.01	K	Joback Method
tf	332.72	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.96	J/mol×K	724.35	Joback Method
cpg	278.01	J/mol×K	541.02	Joback Method
cpg	290.70	J/mol×K	577.69	Joback Method
cpg	302.62	J/mol×K	614.35	Joback Method
cpg	313.78	J/mol×K	651.02	Joback Method
cpg	324.22	J/mol×K	687.68	Joback Method
cpg	343.05	J/mol×K	761.01	Joback Method
hfust	28.93	kJ/mol	424.00	NIST Webbook
hsubt	99.00	kJ/mol	340.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography: https://www.doi.org/10.1021/je300152t

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=C103899&Units=SI

Legend

chs: Standard solid enthalpy of combustion

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume