

Acetamide, N-(4-methoxyphenyl)-

Other names:	4'-Methoxyacetanilide
	4-(Acetylamino)anisole
	4-Methoxyacetanilide
	Acetanilide, 4'-methoxy-
	Acetanilide, 4-methoxy
	Aceto-p-anisidide
	Aceto-p-anisidine
	Acetyl-p-anisidine
	Metacetin
	N-(4-Methoxyphenyl)acetamide
	N-(4-Methoxyphenyl)acetic acid amide
	N-(4-methoxyphenyl)ethanamide
	N-(p-Methoxyphenyl)acetamide
	N-Acetyl-p-anisidine
	N-Acetyl-p-methoxyaniline
	NSC 4687
	ethanamide, N-(4-methoxyphenyl)-
	p-Acetanisidide
	p-Acetanisidine
	p-methoxyacetanilide
Inchi:	InChI=1S/C9H11NO2/c1-7(11)10-8-3-5-9(12-2)6-4-8/h3-6H,1-2H3,(H,10,11)
InchiKey:	XVAIDCNLVLTVFM-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	COc1ccc(NC(C)=O)cc1
Mol. weight [g/mol]:	165.19

Physical Properties

Property code	Value	Unit	Source
hf	-267.93	kJ/mol	Cheméo Relay (1.0)
hfus	25.40	kJ/mol	Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography
hvap	74.07	kJ/mol	Cheméo Relay (1.0)
ie	8.10 ± 0.20	eV	NIST Webbook
log10ws	-1.30		Aqueous Solubility Prediction Method

logp	1.654		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
rinpol	1648.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	568.70	K	Cheméo Relay (1.0)
tc	787.12	K	Cheméo Relay (1.0)
tf	400.30 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.19	J/mol×K	563.44	Joback Method
cpg	313.64	J/mol×K	599.68	Joback Method
cpg	325.37	J/mol×K	635.91	Joback Method
cpg	336.41	J/mol×K	672.15	Joback Method
cpg	346.75	J/mol×K	708.38	Joback Method
cpg	356.42	J/mol×K	744.62	Joback Method
cpg	365.43	J/mol×K	780.85	Joback Method
hfust	27.82	kJ/mol	400.30	NIST Webbook
hfust	27.82	kJ/mol	400.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je300152t
NIST Webbook:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51661&Units=SI
	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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