Methacetin

Other names:	4'-Methoxyacetanilide 4-(Acetylamino)anisole 4-Methoxyacetanilide Acetamide, N-(4-methoxyphenyl)- 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
CAS:	51-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-16.85	kJ/mol	Joback Method
hf	-195.36	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography
hvap	54.16	kJ/mol	Joback Method

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
pc	3431.89	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	563.44	K	Joback Method
tc	780.85	K	Joback Method
tf	400.30 ± 0.50	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51661&Units=SI

Legend

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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