Acetamide, N-(3-methylphenyl)-

Other names:	1-Acetamido-3-methylbenzene
	3'-Methylacetanilide
	3-Acetamidotoluene
	3-Methylacetanilide
	Aceto-m-aminotoluene
	Acetotoluide
	N-(3-Methylphenyl)acetamide
	N-(3-Tolyl)acetic acid amide
	N-Acetyl-3-methylaniline
	N-Acetyl-m-toluidine
	N-m-Tolylacetamide
	NSC 3103
	m-Acetotoluide
	m-Acetotoluidide
	m-Acetotoluidine
	m-Methylacetanilide
	m-Tolylacetamide
	meta-Acetotoluidide
Inchi:	InChI=1S/C9H11NO/c1-7-4-3-5-9(6-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)
InchiKey:	ALMHSXDYCFOZQD-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CC(=O)Nc1cccc(C)c1
Mol. weight [g/mol]:	149.19
CAS:	537-92-8

Physical Properties

Property code	Value	Unit	Source
chs	-4922.43	kJ/mol	NIST Webbook
gf	88.15	kJ/mol	Joback Method
hf	-63.14	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	51.75	kJ/mol	Joback Method
ie	8.30 ± 0.20	eV	NIST Webbook
log10ws	-2.09		Aqueous Solubility Prediction Method
logp	1.953		Crippen Method
mcvol	125.460	ml/mol	McGowan Method

pc	3501.28	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	576.20	K	NIST Webbook
tc	761.01	K	Joback Method
tf	338.40	K	Aqueous Solubility Prediction Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	333.96	J/mol×K	724.35	Joback Method
cpg	343.05	J/mol×K	761.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.70	K	1.90	NIST Webbook

Sources

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=C537928&Units=SI

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

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume