

Acetamide, N-(2-methylphenyl)-

Other names:	o-Acetotoluidide o-Acetotoluide o-Methylacetanilide N-Acetyl-o-toluidine 2'-Methylacetanilide Acetyl-o-toluidine Acet-o-toluidide 2-Methylacetanilide N-o-Tolylacetamide N-Acetyl-2-toluidine NSC 3365
Inchi:	InChI=1S/C9H11NO/c1-7-5-3-4-6-9(7)10-8(2)11/h3-6H,1-2H3,(H,10,11)
InchiKey:	BPEXTIMJLDWDTL-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CC(=O)Nc1ccccc1C
Mol. weight [g/mol]:	149.19
CAS:	120-66-1

Physical Properties

Property code	Value	Unit	Source
chs	-4871.35 ± 0.79	kJ/mol	NIST Webbook
chs	-4921.97	kJ/mol	NIST Webbook
gf	88.15	kJ/mol	Joback Method
hf	-63.14	kJ/mol	Joback Method
hfs	-242.43 ± 0.79	kJ/mol	NIST Webbook
hfus	19.42	kJ/mol	Joback Method
hvap	51.75	kJ/mol	Joback Method
ie	8.34	eV	NIST Webbook
ie	8.03 ± 0.02	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	1.953		Crippen Method
mvol	125.460	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	569.20	K	NIST Webbook
tc	761.01	K	Joback Method
tf	332.72	K	Joback Method
vc	0.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.22	J/mol×K	687.68	Joback Method
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	343.05	J/mol×K	761.01	Joback Method
hfust	21.70	kJ/mol	382.70	NIST Webbook
hsubt	96.80	kJ/mol	327.50	NIST Webbook

Sources

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=C120661&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

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
hfs:	Solid phase 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

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