

Butanamide, N-(2-methylphenyl)-3-oxo-

Other names:

o-Acetoacetotoluidide
Acetoacetyl-2-methylanilide
2-Acetoacetylaminotoluene
2'-Methylacetoacetanilide
ortho-Acetoacetotoluidide
Acetoacet-o-toluidide
2-Acetoacetotoluidide
N-Acetoacetyl-o-toluidine
Acetoacet-o-toluidine
Acetoacet-ortho-toluidide
NSC 7655

Inchi:

InChI=1S/C11H13NO2/c1-8-5-3-4-6-10(8)12-11(14)7-9(2)13/h3-6H,7H2,1-2H3,(H,12,14)

InchiKey:

TVZIWRMELPWPPR-UHFFFAOYSA-N

Formula:

C11H13NO2

SMILES:

CC(=O)CC(O)=Nc1ccccc1C

Mol. weight [g/mol]:

191.23

CAS:

93-68-5

Physical Properties

Property code	Value	Unit	Source
hf	-237.69	kJ/mol	Joback Method
hvap	69.84	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.562		Crippen Method
mvol	155.210	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
tb	705.35	K	Joback Method
tc	920.44	K	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

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=C93685&Units=SI>

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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