

# Toluidide, 4'-chloro-o-acetoaceto-

<b>Other names:</b>	4'-chloro-2'-methylacetoacetanilide
<b>Inchi:</b>	InChI=1S/C11H12ClNO2/c1-7-5-9(12)3-4-10(7)13-11(15)6-8(2)14/h3-5H,6H2,1-2H3,(H,1
<b>InchiKey:</b>	ODFRAIZRJMUPCP-UHFFFAOYSA-N
<b>Formula:</b>	C11H12ClNO2
<b>SMILES:</b>	CC(=O)CC(=O)Nc1ccc(Cl)cc1C
<b>Mol. weight [g/mol]:</b>	225.67
<b>CAS:</b>	20139-55-3

## Physical Properties

Property code	Value	Unit	Source
gf	-45.49	kJ/mol	Joback Method
hf	-244.21	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	67.99	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.566		Crippen Method
mcvol	167.450	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	683.06	K	Joback Method
tc	906.69	K	Joback Method
tf	447.63	K	Joback Method
vc	0.639	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.69	J/molxK	683.06	Joback Method
cpg	421.42	J/molxK	720.33	Joback Method
cpg	432.33	J/molxK	757.60	Joback Method
cpg	442.45	J/molxK	794.88	Joback Method
cpg	451.81	J/molxK	832.15	Joback Method
cpg	460.45	J/molxK	869.42	Joback Method
cpg	468.40	J/molxK	906.69	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20139553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20139553&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/112-905-2/Toluidide-4-chloro-o-acetoaceto.pdf>

Generated by Cheméo on 2024-04-26 21:59:52.311957891 +0000 UTC m=+16458041.232535202.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.