

# N-acetyl-2-ethoxy-5-chloro aniline

<b>Inchi:</b>	InChI=1S/C10H12ClNO2/c1-3-14-10-5-4-8(11)6-9(10)12-7(2)13/h4-6H,3H2,1-2H3,(H,12,
<b>InchiKey:</b>	GFLADJWUPYTLDK-UHFFFAOYSA-N
<b>Formula:</b>	C10H12ClNO2
<b>SMILES:</b>	CCOc1ccc(Cl)cc1NC(C)=O
<b>Mol. weight [g/mol]:</b>	213.66
<b>CAS:</b>	53689-25-1

## Physical Properties

Property code	Value	Unit	Source
gf	-29.99	kJ/mol	Joback Method
hf	-243.21	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	61.43	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.697		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
tb	628.73	K	Joback Method
tc	847.09	K	Joback Method
tf	408.66	K	Joback Method
vc	0.596	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.92	J/molxK	628.73	Joback Method
cpg	384.13	J/molxK	665.12	Joback Method
cpg	395.60	J/molxK	701.52	Joback Method
cpg	406.35	J/molxK	737.91	Joback Method
cpg	416.38	J/molxK	774.30	Joback Method
cpg	425.71	J/molxK	810.70	Joback Method
cpg	434.34	J/molxK	847.09	Joback Method

# Sources

<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=C53689251&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53689251&amp;Units=SI</a>
<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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvap:</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

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