

# Aniline, 3,4-diethoxy-

<b>Inchi:</b>	InChI=1S/C10H15NO2/c1-3-12-9-6-5-8(11)7-10(9)13-4-2/h5-7H,3-4,11H2,1-2H3
<b>InchiKey:</b>	IKYZLUA AOLUOFW-UHFFFAOYSA-N
<b>Formula:</b>	C10H15NO2
<b>SMILES:</b>	CCOc1ccc(N)cc1OCC
<b>Mol. weight [g/mol]:</b>	181.23
<b>CAS:</b>	39052-12-5

## Physical Properties

Property code	Value	Unit	Source
gf	-17.08	kJ/mol	Joback Method
hf	-266.79	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	56.92	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.066		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	582.21	K	Joback Method
tc	795.30	K	Joback Method
tf	381.64	K	Joback Method
vc	0.552	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.65	J/molxK	582.21	Joback Method
cpg	378.45	J/molxK	617.72	Joback Method
cpg	391.58	J/molxK	653.24	Joback Method
cpg	404.04	J/molxK	688.75	Joback Method
cpg	415.81	J/molxK	724.27	Joback Method
cpg	426.90	J/molxK	759.78	Joback Method
cpg	437.30	J/molxK	795.30	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=C39052125&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39052125&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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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