

# N,N-Diethyl-O-nitroaniline

<b>Inchi:</b>	InChI=1S/C10H14N2O2/c1-3-11(4-2)9-7-5-6-8-10(9)12(13)14/h5-8H,3-4H2,1-2H3
<b>InchiKey:</b>	BUBRUAQVAPTGHV-UHFFFAOYSA-N
<b>Formula:</b>	C10H14N2O2
<b>SMILES:</b>	CCN(CC)c1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	194.23
<b>CAS:</b>	2216-17-3

## Physical Properties

Property code	Value	Unit	Source
gf	282.43	kJ/mol	Joback Method
hf	32.10	kJ/mol	Joback Method
hfus	29.69	kJ/mol	Joback Method
hvap	59.43	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.441		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	624.14	K	Joback Method
tc	854.90	K	Joback Method
tf	417.48	K	Joback Method
vc	0.588	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.46	J/molxK	624.14	Joback Method
cpg	408.90	J/molxK	662.60	Joback Method
cpg	422.31	J/molxK	701.06	Joback Method
cpg	434.76	J/molxK	739.52	Joback Method
cpg	446.29	J/molxK	777.98	Joback Method
cpg	456.97	J/molxK	816.44	Joback Method
cpg	466.85	J/molxK	854.90	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=C2216173&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216173&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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