

# nonyl 4-aminobenzoate

<b>Inchi:</b>	InChI=1S/C16H25NO2/c1-2-3-4-5-6-7-8-13-19-16(18)14-9-11-15(17)12-10-14/h9-12H,2-
<b>InchiKey:</b>	KKGIDNSPWHBLLE-UHFFFAOYSA-N
<b>Formula:</b>	C16H25NO2
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1ccc(N)cc1
<b>Mol. weight [g/mol]:</b>	263.38
<b>CAS:</b>	37139-21-2

## Physical Properties

Property code	Value	Unit	Source
gf	19.15	kJ/mol	Joback Method
hf	-359.52	kJ/mol	Joback Method
hfus	38.83	kJ/mol	Joback Method
hvap	73.95	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.176		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
tb	745.96	K	Joback Method
tc	949.56	K	Joback Method
tf	341.00 ± 1.00	K	NIST Webbook
vc	0.876	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.27	J/molxK	745.96	Joback Method
cpg	685.30	J/molxK	779.89	Joback Method
cpg	700.35	J/molxK	813.83	Joback Method
cpg	714.44	J/molxK	847.76	Joback Method
cpg	727.61	J/molxK	881.69	Joback Method
cpg	739.88	J/molxK	915.63	Joback Method
cpg	751.29	J/molxK	949.56	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<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=C37139212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37139212&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>h vap:</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>m cvol:</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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