

# Phenylacetamide, N-(2-ethylhexyl)-

<b>Inchi:</b>	InChI=1S/C16H25NO/c1-3-5-9-14(4-2)13-17-16(18)12-15-10-7-6-8-11-15/h6-8,10-11,14
<b>InchiKey:</b>	QBPUOUIZPYGRRQ-UHFFFAOYSA-N
<b>Formula:</b>	C16H25NO
<b>SMILES:</b>	CCCCC(CC)CN=C(O)Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	247.38

## Physical Properties

Property code	Value	Unit	Source
hf	-222.12	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.402		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	760.46	K	Joback Method
tc	960.33	K	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=U407227&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407227&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>hf:</b>	Enthalpy of formation 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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