

# Ethyl

## 2-(methylamino)-1-phenyl-3-cyclohexene-1-carboxylate

Other names: Nortilidin

Nortilidine

Inchi: InChI=1S/C16H21NO2/c1-3-19-15(18)16(13-9-5-4-6-10-13)12-8-7-11-14(16)17-2/h4-7,9

InchiKey: PDJZPNKVLDWEKI-UHFFFAOYSA-N

Formula: C16H21NO2

SMILES: CCOC(=O)C1(c2ccccc2)CCC=CC1NC

Mol. weight [g/mol]: 259.34

CAS: 38677-94-0

## Physical Properties

Property code	Value	Unit	Source
gf	92.93	kJ/mol	Joback Method
hf	-221.37	kJ/mol	Joback Method
hfus	26.95	kJ/mol	Joback Method
hvap	68.34	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.425		Crippen Method
mcvol	214.800	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpwl	1859.50		NIST Webbook
rinpwl	1859.50		NIST Webbook
tb	732.90	K	Joback Method
tc	967.20	K	Joback Method
tf	449.12	K	Joback Method
vc	0.798	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.46	J/mol×K	732.90	Joback Method
cpg	644.23	J/mol×K	771.95	Joback Method
cpg	661.97	J/mol×K	811.00	Joback Method
cpg	678.85	J/mol×K	850.05	Joback Method
cpg	695.02	J/mol×K	889.10	Joback Method

cpg	710.63	J/mol×K	928.15	Joback Method
cpg	725.85	J/mol×K	967.20	Joback Method

## Sources

<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>
<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=C38677940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38677940&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>hvac:</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>mccvol:</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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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