

# (2E,4E)-N-Isobutyldodeca-2,4-dienamide

<b>Inchi:</b>	InChI=1S/C16H29NO/c1-4-5-6-7-8-9-10-11-12-13-16(18)17-14-15(2)3/h10-13,15H,4-9,1
<b>InchiKey:</b>	BBRMJCAPNGJKEM-AQASXUMVSA-N
<b>Formula:</b>	C16H29NO
<b>SMILES:</b>	CCCCCCCC=CC=CC(O)=NCC(C)C
<b>Mol. weight [g/mol]:</b>	251.41
<b>CAS:</b>	24738-51-0

## Physical Properties

Property code	Value	Unit	Source
hf	-224.21	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	5.072		Crippen Method
mcvol	239.250	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2153.40		NIST Webbook
rinpol	2153.40		NIST Webbook
rinpol	2142.00		NIST Webbook
rinpol	2142.00		NIST Webbook
tb	742.10	K	Joback Method
tc	927.31	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=C24738510&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24738510&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>
<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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r<sub>inpol</sub>:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/82-333-1/2E-4E-N-Isobutyldodeca-2-4-dienamide.pdf>

Generated by Cheméo on 2024-05-12 19:35:02.710660787 +0000 UTC m=+17831751.631238100.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.