

# N-Isobutyl-11-(3,4-methylenedioxyphenyl)-2E,4E,10E,12E,14E,16E,18E,20E,22E,24E,26E,28E,30E,32E,34E,36E,38E,40E,42E,44E,46E,48E,50E,52E,54E,56E,58E,60E,62E,64E,66E,68E,70E,72E,74E,76E,78E,80E,82E,84E,86E,88E,90E,92E,94E,96E,98E,100E-undecanamide

Other names:  
amide

(2E,4E,10E)-11-(Benzo[d][1,3]dioxol-5-yl)-N-isobutylundeca-2,4,10-trienamide

Inchi: InChI=1S/C22H29NO3/c1-18(2)16-23-22(24)12-10-8-6-4-3-5-7-9-11-19-13-14-20-21(15-

InchiKey: RPOYGOULCHMVBB-ADDDGJNWSA-N

Formula: C22H29NO3

SMILES: CC(C)CN=C(O)C=CC=CCCCC=Cc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 355.47

CAS: 54794-74-0

## Physical Properties

Property code	Value	Unit	Source
hf	-188.10	kJ/mol	Joback Method
hvap	96.97	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.714		Crippen Method
mcvol	296.610	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinqol	2786.80		NIST Webbook
rinqol	2786.80		NIST Webbook
tb	985.49	K	Joback Method
tc	1211.44	K	Joback Method

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54794740&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method: [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

## Legend

<b>hf:</b>	Enthalpy of formation 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinsol:</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/87-110-3/N-Isobutyl-11-3-4-methylenedioxyphenyl-2E-4E-10E-undecatrienoic-amide.p>

Generated by Cheméo on 2024-04-23 06:42:08.466588231 +0000 UTC m=+16143777.387165547.

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