

# Isophthalic acid, monoamide, N-butyl-, hexyl ester

<b>Inchi:</b>	InChI=1S/C18H27NO3/c1-3-5-7-8-13-22-18(21)16-11-9-10-15(14-16)17(20)19-12-6-4-2/
<b>InchiKey:</b>	UTNNEVUSPMWSDJ-UHFFFAOYSA-N
<b>Formula:</b>	C18H27NO3
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(O)=NCCCC)c1
<b>Mol. weight [g/mol]:</b>	305.41

## Physical Properties

Property code	Value	Unit	Source
hf	-514.39	kJ/mol	Joback Method
hvap	87.83	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.528		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	887.93	K	Joback Method
tc	1094.74	K	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=U345812&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345812&amp;Units=SI</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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