

# Isophthalic acid, nonyl tridec-2-ynyl ester

<b>Inchi:</b>	InChI=1S/C30H46O4/c1-3-5-7-9-11-12-13-14-16-18-20-25-34-30(32)28-23-21-22-27(26-
<b>InchiKey:</b>	SLQBTALBQCUELL-UHFFFAOYSA-N
<b>Formula:</b>	C30H46O4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCCCCCCC)c1
<b>Mol. weight [g/mol]:</b>	470.68

## Physical Properties

Property code	Value	Unit	Source
gf	39.46	kJ/mol	Joback Method
hf	-654.77	kJ/mol	Joback Method
hfus	75.80	kJ/mol	Joback Method
hvap	105.78	kJ/mol	Joback Method
log10ws	-10.12		Crippen Method
logp	8.285		Crippen Method
mvol	416.080	ml/mol	McGowan Method
pc	802.51	kPa	Joback Method
rinpol	3587.00		NIST Webbook
rinpol	3587.00		NIST Webbook
tb	1079.04	K	Joback Method
tc	1327.07	K	Joback Method
tf	717.22	K	Joback Method
vc	1.617	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1437.85	J/molxK	1079.04	Joback Method
cpg	1455.02	J/molxK	1120.38	Joback Method
cpg	1470.30	J/molxK	1161.72	Joback Method
cpg	1483.76	J/molxK	1203.06	Joback Method
cpg	1495.48	J/molxK	1244.40	Joback Method
cpg	1505.55	J/molxK	1285.73	Joback Method
cpg	1514.06	J/molxK	1327.07	Joback Method

# Sources

<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=U343921&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343921&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>rinpola:</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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