

# Isophthalic acid, octyl tridec-2-ynyl ester

**Inchi:** InChI=1S/C29H44O4/c1-3-5-7-9-11-12-13-14-15-17-19-24-33-29(31)27-22-20-21-26(25-  
**InchiKey:** NFCVXSVTYWSRAZ-UHFFFAOYSA-N  
**Formula:** C29H44O4  
**SMILES:** CCCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCCCCCCC)c1  
**Mol. weight [g/mol]:** 456.66

## Physical Properties

Property code	Value	Unit	Source
gf	31.04	kJ/mol	Joback Method
hf	-634.13	kJ/mol	Joback Method
hfus	73.21	kJ/mol	Joback Method
hvap	103.55	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	7.895		Crippen Method
mvol	401.990	ml/mol	McGowan Method
pc	848.01	kPa	Joback Method
rinpol	3480.00		NIST Webbook
rinpol	3480.00		NIST Webbook
tb	1056.16	K	Joback Method
tc	1295.83	K	Joback Method
tf	705.95	K	Joback Method
vc	1.562	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1374.73	J/molxK	1056.16	Joback Method
cpg	1391.64	J/molxK	1096.11	Joback Method
cpg	1406.78	J/molxK	1136.05	Joback Method
cpg	1420.22	J/molxK	1176.00	Joback Method
cpg	1432.02	J/molxK	1215.94	Joback Method
cpg	1442.27	J/molxK	1255.89	Joback Method
cpg	1451.03	J/molxK	1295.83	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U343920&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343920&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>hvp:</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>rinp:</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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