

# Isophthalic acid, isoheptyl tridec-2-ynyl ester

**Inchi:** InChI=1S/C27H40O4/c1-4-5-6-7-8-9-10-11-12-13-14-20-30-26(28)24-18-15-19-25(22-24)  
**InchiKey:** PVYMYZRUBTUZDZ-UHFFFAOYSA-N  
**Formula:** C27H40O4  
**SMILES:** CCCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1  
**Mol. weight [g/mol]:** 428.60

## Physical Properties

Property code	Value	Unit	Source
gf	11.76	kJ/mol	Joback Method
hf	-598.13	kJ/mol	Joback Method
hfus	64.51	kJ/mol	Joback Method
hvap	98.71	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	6.971		Crippen Method
mvol	373.810	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		NIST Webbook
tb	1009.96	K	Joback Method
tc	1236.49	K	Joback Method
tf	668.41	K	Joback Method
vc	1.444	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.77	J/molxK	1009.96	Joback Method
cpg	1266.16	J/molxK	1047.71	Joback Method
cpg	1280.98	J/molxK	1085.47	Joback Method
cpg	1294.27	J/molxK	1123.22	Joback Method
cpg	1306.09	J/molxK	1160.98	Joback Method
cpg	1316.49	J/molxK	1198.73	Joback Method
cpg	1325.52	J/molxK	1236.49	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U343917&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343917&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>
<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>

# 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>hvpap:</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>rinppl:</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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