

# Isophthalic acid, 2,7-dimethyloct-7-en-5-yn-4-yl isoheptyl ester

Inchi:	InChI=1S/C24H32O4/c1-17(2)9-8-14-27-23(25)20-10-7-11-21(16-20)24(26)28-22(15-19)
InchiKey:	RCRDNQVBUCCUPR-UHFFFAOYSA-N
Formula:	C24H32O4
SMILES:	<chem>C=C(C)C#CC(CC(C)C)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1</chem>
Mol. weight [g/mol]:	384.51

## Physical Properties

Property code	Value	Unit	Source
gf	60.91	kJ/mol	Joback Method
hf	-431.13	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.431		Crippen Method
mvol	327.240	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	937.00	K	Joback Method
tc	1158.44	K	Joback Method
tf	588.88	K	Joback Method
vc	1.246	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.46	J/molxK	937.00	Joback Method
cpg	1052.32	J/molxK	973.91	Joback Method
cpg	1066.79	J/molxK	1010.81	Joback Method
cpg	1079.92	J/molxK	1047.72	Joback Method
cpg	1091.75	J/molxK	1084.62	Joback Method
cpg	1102.33	J/molxK	1121.53	Joback Method
cpg	1111.70	J/molxK	1158.44	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=U343849&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343849&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>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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