

# Isophthalic acid, octadecyl neopentyl ester

<b>Inchi:</b>	InChI=1S/C31H52O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-34-29(32)27-2
<b>InchiKey:</b>	GVWPTIXNSPJKAF-UHFFFAOYSA-N
<b>Formula:</b>	C31H52O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
<b>Mol. weight [g/mol]:</b>	488.74

## Physical Properties

Property code	Value	Unit	Source
gf	-152.08	kJ/mol	Joback Method
hf	-956.46	kJ/mol	Joback Method
hfus	67.86	kJ/mol	Joback Method
hvap	104.55	kJ/mol	Joback Method
log10ws	-10.51		Crippen Method
logp	9.308		Crippen Method
mvol	438.770	ml/mol	McGowan Method
pc	704.71	kPa	Joback Method
rinpol	3569.00		NIST Webbook
rinpol	3569.00		NIST Webbook
tb	1089.69	K	Joback Method
tc	1347.99	K	Joback Method
tf	624.81	K	Joback Method
vc	1.700	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.03	J/molxK	1089.69	Joback Method
cpg	1641.25	J/molxK	1304.94	Joback Method
cpg	1628.42	J/molxK	1261.89	Joback Method
cpg	1614.12	J/molxK	1218.84	Joback Method
cpg	1598.22	J/molxK	1175.79	Joback Method
cpg	1580.57	J/molxK	1132.74	Joback Method
cpg	1652.77	J/molxK	1347.99	Joback Method
dvisc	0.0000077	Paxs	1089.69	Joback Method

dvisc	0.0000103	Paxs	1012.21	Joback Method
dvisc	0.0000146	Paxs	934.73	Joback Method
dvisc	0.0000219	Paxs	857.25	Joback Method
dvisc	0.0000355	Paxs	779.77	Joback Method
dvisc	0.0000642	Paxs	702.29	Joback Method
dvisc	0.0001346	Paxs	624.81	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U343874&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343874&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>dvisc:</b>	Dynamic viscosity
<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>mccvol:</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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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