

# Isophthalic acid, neopentyl pentyl ester

<b>Inchi:</b>	InChI=1S/C18H26O4/c1-5-6-7-11-21-16(19)14-9-8-10-15(12-14)17(20)22-13-18(2,3)4/h8
<b>InchiKey:</b>	ANFABKSQZPSEOC-UHFFFAOYSA-N
<b>Formula:</b>	C18H26O4
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
<b>Mol. weight [g/mol]:</b>	306.40

## Physical Properties

Property code	Value	Unit	Source
gf	-261.54	kJ/mol	Joback Method
hf	-688.14	kJ/mol	Joback Method
hfus	34.19	kJ/mol	Joback Method
hvap	75.62	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.237		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	792.25	K	Joback Method
tc	998.90	K	Joback Method
tf	478.30	K	Joback Method
vc	0.973	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.82	J/molxK	792.25	Joback Method
cpg	831.80	J/molxK	964.46	Joback Method
cpg	820.07	J/molxK	930.02	Joback Method
cpg	807.34	J/molxK	895.58	Joback Method
cpg	793.58	J/molxK	861.13	Joback Method
cpg	778.75	J/molxK	826.69	Joback Method
cpg	842.58	J/molxK	998.90	Joback Method
dvisc	0.0000580	Paxs	792.25	Joback Method

dvisc	0.0000756	Paxs	739.92	Joback Method
dvisc	0.0001025	Paxs	687.60	Joback Method
dvisc	0.0001462	Paxs	635.27	Joback Method
dvisc	0.0002223	Paxs	582.95	Joback Method
dvisc	0.0003670	Paxs	530.62	Joback Method
dvisc	0.0006763	Paxs	478.30	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=U343862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343862&amp;Units=SI</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>mcvol:</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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