

# Isophthalic acid, cyclohexylmethyl undecyl ester

Inchi:	InChI=1S/C26H40O4/c1-2-3-4-5-6-7-8-9-13-19-29-25(27)23-17-14-18-24(20-23)26(28)30
InchiKey:	WLBYQABGVLTJEW-UHFFFAOYSA-N
Formula:	C26H40O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	416.59

## Physical Properties

Property code	Value	Unit	Source
gf	-172.57	kJ/mol	Joback Method
hf	-790.19	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	95.15	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.111		Crippen Method
mvol	357.460	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
rinpol	3291.00		NIST Webbook
rinpol	3291.00		NIST Webbook
tb	998.07	K	Joback Method
tc	1223.03	K	Joback Method
tf	573.42	K	Joback Method
vc	1.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.34	J/molxK	998.07	Joback Method
cpg	1254.97	J/molxK	1035.56	Joback Method
cpg	1269.87	J/molxK	1073.06	Joback Method
cpg	1283.09	J/molxK	1110.55	Joback Method
cpg	1294.70	J/molxK	1148.05	Joback Method
cpg	1304.76	J/molxK	1185.54	Joback Method
cpg	1313.31	J/molxK	1223.03	Joback Method
dvisc	0.0003382	Paxs	573.42	Joback Method

dvisc	0.0001696	Paxs	644.20	Joback Method
dvisc	0.0000975	Paxs	714.97	Joback Method
dvisc	0.0000619	Paxs	785.75	Joback Method
dvisc	0.0000424	Paxs	856.52	Joback Method
dvisc	0.0000308	Paxs	927.29	Joback Method
dvisc	0.0000234	Paxs	998.07	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=U343833&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343833&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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