

# Isophthalic acid, 2-methylcyclohexyl undecyl ester

Inchi:	InChI=1S/C26H40O4/c1-3-4-5-6-7-8-9-10-13-19-29-25(27)22-16-14-17-23(20-22)26(28)3
InchiKey:	NWLKURLKARMJMS-UHFFFAOYSA-N
Formula:	C26H40O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]:	416.59

## Physical Properties

Property code	Value	Unit	Source
gf	-180.28	kJ/mol	Joback Method
hf	-810.53	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	94.84	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.110		Crippen Method
mvol	357.460	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	3194.00		NIST Webbook
rinpol	3194.00		NIST Webbook
tb	993.40	K	Joback Method
tc	1217.53	K	Joback Method
tf	569.18	K	Joback Method
vc	1.363	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.81	J/molxK	993.40	Joback Method
cpg	1308.91	J/molxK	1180.18	Joback Method
cpg	1299.12	J/molxK	1142.82	Joback Method
cpg	1287.67	J/molxK	1105.47	Joback Method
cpg	1274.49	J/molxK	1068.11	Joback Method
cpg	1259.56	J/molxK	1030.76	Joback Method
cpg	1317.07	J/molxK	1217.53	Joback Method
dvisc	0.0000314	Paxs	993.40	Joback Method

dvisc	0.0000407	Paxs	922.70	Joback Method
dvisc	0.0000550	Paxs	851.99	Joback Method
dvisc	0.0000786	Paxs	781.29	Joback Method
dvisc	0.0001205	Paxs	710.59	Joback Method
dvisc	0.0002030	Paxs	639.88	Joback Method
dvisc	0.0003892	Paxs	569.18	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=U345755&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345755&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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