

# Isophthalic acid, dodecyl 1-propylbutyl ester

<b>Inchi:</b>	InChI=1S/C27H44O4/c1-4-7-8-9-10-11-12-13-14-15-21-30-26(28)23-19-16-20-24(22-23)
<b>InchiKey:</b>	SFHPZLLDWSMLHF-UHFFFAOYSA-N
<b>Formula:</b>	C27H44O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCC)c1
<b>Mol. weight [g/mol]:</b>	432.64

## Physical Properties

Property code	Value	Unit	Source
gf	-191.04	kJ/mol	Joback Method
hf	-870.43	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	96.56	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	7.890		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	868.11	kPa	Joback Method
rinsol	2996.00		NIST Webbook
tb	1000.96	K	Joback Method
tc	1226.87	K	Joback Method
tf	562.31	K	Joback Method
vc	1.482	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.77	J/molxK	1000.96	Joback Method
cpg	1379.63	J/molxK	1189.22	Joback Method
cpg	1368.14	J/molxK	1151.57	Joback Method
cpg	1355.17	J/molxK	1113.92	Joback Method
cpg	1340.65	J/molxK	1076.26	Joback Method
cpg	1324.54	J/molxK	1038.61	Joback Method
cpg	1389.70	J/molxK	1226.87	Joback Method
dvisc	0.0000178	Paxs	1000.96	Joback Method
dvisc	0.0000236	Paxs	927.85	Joback Method

dvisc	0.0000330	Paxs	854.74	Joback Method
dvisc	0.0000489	Paxs	781.63	Joback Method
dvisc	0.0000788	Paxs	708.53	Joback Method
dvisc	0.0001415	Paxs	635.42	Joback Method
dvisc	0.0002962	Paxs	562.31	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=U356407&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356407&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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