

# Isophthalic acid, dodecyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C26H40O4/c1-3-5-7-9-10-11-12-13-14-16-21-30-26(28)24-19-17-18-23(22-24)
InchiKey:	KTVGKSFJJUMFRS-SOFGYWHQSA-N
Formula:	C26H40O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCC)c1
Mol. weight [g/mol]:	416.59

## Physical Properties

Property code	Value	Unit	Source
gf	-116.80	kJ/mol	Joback Method
hf	-727.29	kJ/mol	Joback Method
hfus	62.52	kJ/mol	Joback Method
hvap	94.68	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mvol	364.020	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	982.68	K	Joback Method
tc	1203.15	K	Joback Method
tf	560.96	K	Joback Method
vc	1.411	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.28	J/molxK	982.68	Joback Method
cpg	1232.52	J/molxK	1019.43	Joback Method
cpg	1248.39	J/molxK	1056.17	Joback Method
cpg	1262.94	J/molxK	1092.92	Joback Method
cpg	1276.23	J/molxK	1129.66	Joback Method
cpg	1288.35	J/molxK	1166.41	Joback Method
cpg	1299.34	J/molxK	1203.15	Joback Method
dvisc	0.0002809	Paxs	560.96	Joback Method

dvisc	0.0001416	Paxs	631.25	Joback Method
dvisc	0.0000818	Paxs	701.53	Joback Method
dvisc	0.0000523	Paxs	771.82	Joback Method
dvisc	0.0000360	Paxs	842.11	Joback Method
dvisc	0.0000262	Paxs	912.39	Joback Method
dvisc	0.0000200	Paxs	982.68	Joback Method

## Sources

<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=U356695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356695&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>

## 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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