

# Isophthalic acid, cis-hex-3-enyl heptadecyl ester

Inchi:	InChI=1S/C31H50O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-21-26-35-31(33)29-24-
InchiKey:	ZMFVYHBRVIDFJW-VURMDHGXSA-N
Formula:	C31H50O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCCCC)c1
Mol. weight [g/mol]:	486.73

## Physical Properties

Property code	Value	Unit	Source
gf	-74.70	kJ/mol	Joback Method
hf	-830.49	kJ/mol	Joback Method
hfus	75.47	kJ/mol	Joback Method
hvap	105.81	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	9.228		Crippen Method
mcvol	434.470	ml/mol	McGowan Method
pc	717.22	kPa	Joback Method
rinpol	3566.00		NIST Webbook
tb	1097.08	K	Joback Method
tc	1360.33	K	Joback Method
tf	617.31	K	Joback Method
vc	1.692	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.26	J/molxK	1097.08	Joback Method
cpg	1612.02	J/molxK	1316.45	Joback Method
cpg	1599.35	J/molxK	1272.58	Joback Method
cpg	1585.18	J/molxK	1228.70	Joback Method
cpg	1569.37	J/molxK	1184.83	Joback Method
cpg	1551.78	J/molxK	1140.95	Joback Method
cpg	1623.33	J/molxK	1360.33	Joback Method
dvisc	0.0000092	Paxs	1097.08	Joback Method
dvisc	0.0000122	Paxs	1017.12	Joback Method

dvisc	0.0000169	Paxs	937.16	Joback Method
dvisc	0.0000250	Paxs	857.19	Joback Method
dvisc	0.0000401	Paxs	777.23	Joback Method
dvisc	0.0000716	Paxs	697.27	Joback Method
dvisc	0.0001483	Paxs	617.31	Joback Method

## Sources

<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=U356711&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356711&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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