

# Isophthalic acid, isobutyl 2-hexyl ester

<b>Other names:</b>	Isophthalic acid, hex-3-yl isobutyl ester
<b>Inchi:</b>	InChI=1S/C19H28O4/c1-5-6-7-9-15(4)23-19(21)17-11-8-10-16(12-17)18(20)22-13-14(2)3
<b>InchiKey:</b>	GIEIKRSFYHPDNL-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O4
<b>SMILES:</b>	CCCCCC(C)OC(=O)c1cccc(C(=O)OCC(C)C)c1
<b>Mol. weight [g/mol]:</b>	320.42

## Physical Properties

Property code	Value	Unit	Source
gf	-260.84	kJ/mol	Joback Method
hf	-710.59	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.625		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	817.48	K	Joback Method
tc	1021.25	K	Joback Method
tf	457.15	K	Joback Method
vc	1.028	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.12	J/mol×K	817.48	Joback Method
cpg	836.35	J/mol×K	851.44	Joback Method
cpg	851.44	J/mol×K	885.40	Joback Method
cpg	865.39	J/mol×K	919.36	Joback Method
cpg	878.23	J/mol×K	953.32	Joback Method
cpg	889.98	J/mol×K	987.28	Joback Method
cpg	900.66	J/mol×K	1021.25	Joback Method

dvisc	0.0008629	Paxs	457.15	Joback Method
dvisc	0.0004138	Paxs	517.21	Joback Method
dvisc	0.0002312	Paxs	577.26	Joback Method
dvisc	0.0001441	Paxs	637.32	Joback Method
dvisc	0.0000975	Paxs	697.37	Joback Method
dvisc	0.0000702	Paxs	757.42	Joback Method
dvisc	0.0000530	Paxs	817.48	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356493&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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

Latest version available from:

<https://www.cheméo.com/cid/27-456-6/Isophthalic-acid-isobutyl-2-hexyl-ester.pdf>

Generated by Cheméo on 2023-09-24 08:07:57.309101685 +0000 UTC m=+911845.224914794.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.