

# Isophthalic acid, 3,5-dimethylcyclohexyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C20H28O4/c1-13(2)12-23-19(21)16-6-5-7-17(11-16)20(22)24-18-9-14(3)8-15(4)
<b>InchiKey:</b>	GIJDEOZGCPXDBG-UHFFFAOYSA-N
<b>Formula:</b>	C20H28O4
<b>SMILES:</b>	CC(C)COC(=O)c1cccc(C(=O)OC2CC(C)CC(C)C2)c1
<b>Mol. weight [g/mol]:</b>	332.43

## Physical Properties

Property code	Value	Unit	Source
gf	-240.95	kJ/mol	Joback Method
hf	-712.31	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	80.79	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.481		Crippen Method
mvol	272.920	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook
tb	851.01	K	Joback Method
tc	1072.70	K	Joback Method
tf	482.32	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.13	J/molxK	851.01	Joback Method
cpg	899.09	J/molxK	887.96	Joback Method
cpg	915.40	J/molxK	924.91	Joback Method
cpg	930.08	J/molxK	961.85	Joback Method
cpg	943.15	J/molxK	998.80	Joback Method
cpg	954.63	J/molxK	1035.75	Joback Method
cpg	964.51	J/molxK	1072.70	Joback Method
dvisc	0.0008820	Paxs	482.32	Joback Method

dvisc	0.0004820	Paxs	543.77	Joback Method
dvisc	0.0002978	Paxs	605.22	Joback Method
dvisc	0.0002011	Paxs	666.66	Joback Method
dvisc	0.0001451	Paxs	728.11	Joback Method
dvisc	0.0001101	Paxs	789.56	Joback Method
dvisc	0.0000870	Paxs	851.01	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=U343820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343820&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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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