

# Isophthalic acid, hex-3-yl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C20H30O4/c1-5-9-18(6-2)24-20(22)17-12-7-11-16(14-17)19(21)23-13-8-10-15
<b>InchiKey:</b>	CHAJOGBOLYAYQU-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O4
<b>SMILES:</b>	CCCC(CC)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
<b>Mol. weight [g/mol]:</b>	334.45

## Physical Properties

Property code	Value	Unit	Source
gf	-252.42	kJ/mol	Joback Method
hf	-731.23	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	80.59	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.015		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	840.36	K	Joback Method
tc	1043.99	K	Joback Method
tf	468.42	K	Joback Method
vc	1.083	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.75	J/molxK	840.36	Joback Method
cpg	949.07	J/molxK	1010.06	Joback Method
cpg	937.29	J/molxK	976.12	Joback Method
cpg	924.40	J/molxK	942.18	Joback Method
cpg	910.36	J/molxK	908.24	Joback Method
cpg	895.15	J/molxK	874.30	Joback Method
cpg	959.75	J/molxK	1043.99	Joback Method
dvisc	0.0000460	Paxs	840.36	Joback Method

dvisc	0.0000611	Paxs	778.37	Joback Method
dvisc	0.0000852	Paxs	716.38	Joback Method
dvisc	0.0001265	Paxs	654.39	Joback Method
dvisc	0.0002040	Paxs	592.40	Joback Method
dvisc	0.0003677	Paxs	530.41	Joback Method
dvisc	0.0007750	Paxs	468.42	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=U356490&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356490&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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