

# Isophthalic acid, 2-cyclohexylethyl isohexyl ester

Inchi:	InChI=1S/C22H32O4/c1-17(2)8-7-14-25-21(23)19-11-6-12-20(16-19)22(24)26-15-13-18-
InchiKey:	UYBHQHCBHFHDKN-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]:	360.49

## Physical Properties

Property code	Value	Unit	Source
gf	-208.69	kJ/mol	Joback Method
hf	-712.91	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.407		Crippen Method
mvol	301.100	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	906.11	K	Joback Method
tc	1126.08	K	Joback Method
tf	513.34	K	Joback Method
vc	1.135	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.13	J/molxK	906.11	Joback Method
cpg	1010.08	J/molxK	942.77	Joback Method
cpg	1025.46	J/molxK	979.43	Joback Method
cpg	1039.30	J/molxK	1016.09	Joback Method
cpg	1051.65	J/molxK	1052.75	Joback Method
cpg	1062.53	J/molxK	1089.41	Joback Method
cpg	1071.99	J/molxK	1126.08	Joback Method
dvisc	0.0006115	Paxs	513.34	Joback Method

dvisc	0.0002980	Paxs	578.80	Joback Method
dvisc	0.0001681	Paxs	644.26	Joback Method
dvisc	0.0001053	Paxs	709.72	Joback Method
dvisc	0.0000714	Paxs	775.19	Joback Method
dvisc	0.0000515	Paxs	840.65	Joback Method
dvisc	0.0000389	Paxs	906.11	Joback Method

## Sources

<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>
<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=U343812&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343812&amp;Units=SI</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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