

# Isophthalic acid, 2-cyclohexylethyl heptyl ester

Inchi:	InChI=1S/C23H34O4/c1-2-3-4-5-9-16-26-22(24)20-13-10-14-21(18-20)23(25)27-17-15-1
InchiKey:	UCVSVXWJYXTQLO-UHFFFAOYSA-N
Formula:	C23H34O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]:	374.51

## Physical Properties

Property code	Value	Unit	Source
gf	-197.83	kJ/mol	Joback Method
hf	-728.27	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	88.47	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.941		Crippen Method
mvol	315.190	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	929.43	K	Joback Method
tc	1147.80	K	Joback Method
tf	539.61	K	Joback Method
vc	1.196	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.39	J/molxK	929.43	Joback Method
cpg	1070.16	J/molxK	965.82	Joback Method
cpg	1085.35	J/molxK	1002.22	Joback Method
cpg	1099.02	J/molxK	1038.61	Joback Method
cpg	1111.19	J/molxK	1075.01	Joback Method
cpg	1121.93	J/molxK	1111.40	Joback Method
cpg	1131.26	J/molxK	1147.80	Joback Method
dvisc	0.0004850	Paxs	539.61	Joback Method

dvisc	0.0002504	Paxs	604.58	Joback Method
dvisc	0.0001470	Paxs	669.55	Joback Method
dvisc	0.0000948	Paxs	734.52	Joback Method
dvisc	0.0000657	Paxs	799.49	Joback Method
dvisc	0.0000481	Paxs	864.46	Joback Method
dvisc	0.0000368	Paxs	929.43	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=U343814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343814&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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