

# Isophthalic acid, 6-chlorohexyl heptyl ester

<b>Inchi:</b>	InChI=1S/C21H31ClO4/c1-2-3-4-6-9-15-25-20(23)18-12-11-13-19(17-18)21(24)26-16-10
<b>InchiKey:</b>	DHRBOFIVNIKSBM-UHFFFAOYSA-N
<b>Formula:</b>	C21H31ClO4
<b>SMILES:</b>	CCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCI)c1
<b>Mol. weight [g/mol]:</b>	382.92

## Physical Properties

Property code	Value	Unit	Source
gf	-251.05	kJ/mol	Joback Method
hf	-757.05	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.770		Crippen Method
mvol	310.110	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	901.55	K	Joback Method
tc	1108.65	K	Joback Method
tf	539.61	K	Joback Method
vc	1.200	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.34	J/molxK	901.55	Joback Method
cpg	979.52	J/molxK	936.07	Joback Method
cpg	993.50	J/molxK	970.58	Joback Method
cpg	1006.30	J/molxK	1005.10	Joback Method
cpg	1017.96	J/molxK	1039.62	Joback Method
cpg	1028.51	J/molxK	1074.14	Joback Method
cpg	1037.97	J/molxK	1108.65	Joback Method
dvisc	0.0004342	Paxs	539.61	Joback Method

dvisc	0.0002402	Paxs	599.93	Joback Method
dvisc	0.0001480	Paxs	660.26	Joback Method
dvisc	0.0000989	Paxs	720.58	Joback Method
dvisc	0.0000704	Paxs	780.90	Joback Method
dvisc	0.0000526	Paxs	841.23	Joback Method
dvisc	0.0000408	Paxs	901.55	Joback Method

## Sources

<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=U345883&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345883&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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