

# Isophthalic acid, 10-chlorodecyl heptyl ester

**Inchi:** InChI=1S/C25H39ClO4/c1-2-3-4-10-13-19-29-24(27)22-16-15-17-23(21-22)25(28)30-20-  
**InchiKey:** TXUGJHMAOXMISD-UHFFFAOYSA-N  
**Formula:** C25H39ClO4  
**SMILES:** CCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCl)c1  
**Mol. weight [g/mol]:** 439.03

## Physical Properties

Property code	Value	Unit	Source
gf	-217.37	kJ/mol	Joback Method
hf	-839.61	kJ/mol	Joback Method
hfus	63.93	kJ/mol	Joback Method
hvap	96.88	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.330		Crippen Method
mvol	366.470	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook
tb	993.07	K	Joback Method
tc	1216.15	K	Joback Method
tf	584.69	K	Joback Method
vc	1.425	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.72	J/molxK	993.07	Joback Method
cpg	1273.94	J/molxK	1178.97	Joback Method
cpg	1263.48	J/molxK	1141.79	Joback Method
cpg	1251.68	J/molxK	1104.61	Joback Method
cpg	1238.49	J/molxK	1067.43	Joback Method
cpg	1223.86	J/molxK	1030.25	Joback Method
cpg	1283.10	J/molxK	1216.15	Joback Method
dvisc	0.0000223	Paxs	993.07	Joback Method

dvisc	0.0000290	Paxs	925.01	Joback Method
dvisc	0.0000394	Paxs	856.94	Joback Method
dvisc	0.0000563	Paxs	788.88	Joback Method
dvisc	0.0000862	Paxs	720.82	Joback Method
dvisc	0.0001441	Paxs	652.75	Joback Method
dvisc	0.0002716	Paxs	584.69	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=U356419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356419&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>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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