

# Phthalic acid, isoheptyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C20H19Cl3O4/c1-12(2)6-5-9-26-19(24)14-7-3-4-8-15(14)20(25)27-13-10-16(2)
InchiKey:	RHFDMLPOUCGTNX-UHFFFAOYSA-N
Formula:	C20H19Cl3O4
SMILES:	CC(C)CCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	429.72

## Physical Properties

Property code	Value	Unit	Source
gf	-202.25	kJ/mol	Joback Method
hf	-571.05	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.459		Crippen Method
mvol	296.740	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	994.71	K	Joback Method
tc	1234.50	K	Joback Method
tf	637.16	K	Joback Method
vc	1.129	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.96	J/molxK	994.71	Joback Method
cpg	876.35	J/molxK	1194.53	Joback Method
cpg	871.87	J/molxK	1154.57	Joback Method
cpg	866.11	J/molxK	1114.60	Joback Method
cpg	859.06	J/molxK	1074.64	Joback Method
cpg	850.69	J/molxK	1034.67	Joback Method
cpg	879.60	J/molxK	1234.50	Joback Method
dvisc	0.0000343	Paxs	994.71	Joback Method

dvisc	0.0000425	Paxs	935.12	Joback Method
dvisc	0.0000543	Paxs	875.53	Joback Method
dvisc	0.0000717	Paxs	815.93	Joback Method
dvisc	0.0000991	Paxs	756.34	Joback Method
dvisc	0.0001446	Paxs	696.75	Joback Method
dvisc	0.0002265	Paxs	637.16	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=U357068&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357068&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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