

# Phthalic acid, heptyl 2,4,6-trichlorobenzyl ester

Inchi:	InChI=1S/C22H23Cl3O4/c1-2-3-4-5-8-11-28-21(26)16-9-6-7-10-17(16)22(27)29-14-18-19
InchiKey:	QXTSLAOGBMQXAT-UHFFFAOYSA-N
Formula:	C22H23Cl3O4
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	457.77

## Physical Properties

Property code	Value	Unit	Source
gf	-182.97	kJ/mol	Joback Method
hf	-607.05	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	103.23	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.131		Crippen Method
mvol	324.920	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		NIST Webbook
tb	1040.91	K	Joback Method
tc	1280.01	K	Joback Method
tf	674.70	K	Joback Method
vc	1.246	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.55	J/molxK	1040.91	Joback Method
cpg	966.37	J/molxK	1080.76	Joback Method
cpg	974.79	J/molxK	1120.61	Joback Method
cpg	981.85	J/molxK	1160.46	Joback Method
cpg	987.59	J/molxK	1200.31	Joback Method
cpg	992.05	J/molxK	1240.16	Joback Method
cpg	995.26	J/molxK	1280.01	Joback Method
dvisc	0.0001729	Paxs	674.70	Joback Method

dvisc	0.0001125	Paxs	735.74	Joback Method
dvisc	0.0000782	Paxs	796.77	Joback Method
dvisc	0.0000572	Paxs	857.80	Joback Method
dvisc	0.0000437	Paxs	918.84	Joback Method
dvisc	0.0000345	Paxs	979.87	Joback Method
dvisc	0.0000280	Paxs	1040.91	Joback Method

## Sources

<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=U382881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382881&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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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