

# Phthalic acid, isobutyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C18H15Cl3O4/c1-10(2)9-24-17(22)11-5-3-4-6-12(11)18(23)25-16-8-14(20)13(
InchiKey:	KYVFGNDKKBKJZIY-UHFFFAOYSA-N
Formula:	C18H15Cl3O4
SMILES:	CC(C)COC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	401.67

## Physical Properties

Property code	Value	Unit	Source
gf	-219.09	kJ/mol	Joback Method
hf	-529.77	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.679		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	948.95	K	Joback Method
tc	1191.57	K	Joback Method
tf	614.62	K	Joback Method
vc	1.016	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.27	J/molxK	948.95	Joback Method
cpg	736.84	J/molxK	989.39	Joback Method
cpg	745.12	J/molxK	1029.82	Joback Method
cpg	752.13	J/molxK	1070.26	Joback Method
cpg	757.88	J/molxK	1110.70	Joback Method
cpg	762.39	J/molxK	1151.13	Joback Method
cpg	765.69	J/molxK	1191.57	Joback Method
dvisc	0.0002812	Paxs	614.62	Joback Method

dvisc	0.0001835	Paxs	670.34	Joback Method
dvisc	0.0001279	Paxs	726.06	Joback Method
dvisc	0.0000938	Paxs	781.79	Joback Method
dvisc	0.0000717	Paxs	837.51	Joback Method
dvisc	0.0000567	Paxs	893.23	Joback Method
dvisc	0.0000461	Paxs	948.95	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=U357043&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357043&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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