

# Phthalic acid, pentyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C19H17Cl3O4/c1-2-3-6-9-25-18(23)13-7-4-5-8-14(13)19(24)26-16-11-12(20)10
InchiKey:	YKJWGFWAUBYIFZ-UHFFFAOYSA-N
Formula:	C19H17Cl3O4
SMILES:	CCCCCOC(=O)c1cccc1C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	415.69

## Physical Properties

Property code	Value	Unit	Source
gf	-208.23	kJ/mol	Joback Method
hf	-545.13	kJ/mol	Joback Method
hfus	49.66	kJ/mol	Joback Method
hvap	96.55	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.213		Crippen Method
mvol	282.650	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2825.00		NIST Webbook
tb	972.27	K	Joback Method
tc	1210.51	K	Joback Method
tf	640.89	K	Joback Method
vc	1.079	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.33	J/molxK	972.27	Joback Method
cpg	792.96	J/molxK	1011.98	Joback Method
cpg	801.32	J/molxK	1051.68	Joback Method
cpg	808.41	J/molxK	1091.39	Joback Method
cpg	814.28	J/molxK	1131.10	Joback Method
cpg	818.93	J/molxK	1170.81	Joback Method
cpg	822.41	J/molxK	1210.51	Joback Method
dvisc	0.0002413	Paxs	640.89	Joback Method
dvisc	0.0001621	Paxs	696.12	Joback Method

dvisc	0.0001155	Paxs	751.35	Joback Method
dvisc	0.0000862	Paxs	806.58	Joback Method
dvisc	0.0000668	Paxs	861.81	Joback Method
dvisc	0.0000533	Paxs	917.04	Joback Method
dvisc	0.0000437	Paxs	972.27	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=U357058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357058&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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