

# Pimelic acid, butyl 2,6-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H22Cl2O4/c1-2-3-12-22-15(20)10-5-4-6-11-16(21)23-17-13(18)8-7-9-14(19)
<b>InchiKey:</b>	SQSQQENBKISEEJ-UHFFFAOYSA-N
<b>Formula:</b>	C17H22Cl2O4
<b>SMILES:</b>	CCCCOC(=O)CCCCC(=O)Oc1c(Cl)cccc1Cl
<b>Mol. weight [g/mol]:</b>	361.26

## Physical Properties

Property code	Value	Unit	Source
gf	-306.29	kJ/mol	Joback Method
hf	-701.70	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.193		Crippen Method
mvol	265.990	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	852.44	K	Joback Method
tc	1062.07	K	Joback Method
tf	536.97	K	Joback Method
vc	1.026	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.26	J/molxK	852.44	Joback Method
cpg	768.31	J/molxK	887.38	Joback Method
cpg	780.32	J/molxK	922.32	Joback Method
cpg	791.29	J/molxK	957.25	Joback Method
cpg	801.26	J/molxK	992.19	Joback Method
cpg	810.22	J/molxK	1027.13	Joback Method
cpg	818.20	J/molxK	1062.07	Joback Method
dvisc	0.0004746	Paxs	536.97	Joback Method

dvisc	0.0002921	Paxs	589.55	Joback Method
dvisc	0.0001947	Paxs	642.13	Joback Method
dvisc	0.0001380	Paxs	694.70	Joback Method
dvisc	0.0001026	Paxs	747.28	Joback Method
dvisc	0.0000794	Paxs	799.86	Joback Method
dvisc	0.0000634	Paxs	852.44	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=U416656&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416656&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>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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