

# Pimelic acid, butyl 3,5-dichlorobenzyl ester

<b>Inchi:</b>	InChI=1S/C18H24Cl2O4/c1-2-3-9-23-17(21)7-5-4-6-8-18(22)24-13-14-10-15(19)12-16(20)
<b>InchiKey:</b>	IYYHFTKDTRFCSN-UHFFFAOYSA-N
<b>Formula:</b>	C18H24Cl2O4
<b>SMILES:</b>	CCCCOC(=O)CCCCC(=O)OCc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	375.29

## Physical Properties

Property code	Value	Unit	Source
gf	-297.87	kJ/mol	Joback Method
hf	-722.34	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.330		Crippen Method
mvol	280.080	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	875.32	K	Joback Method
tc	1084.97	K	Joback Method
tf	548.24	K	Joback Method
vc	1.081	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.47	J/molxK	875.32	Joback Method
cpg	825.76	J/molxK	910.26	Joback Method
cpg	837.96	J/molxK	945.20	Joback Method
cpg	849.09	J/molxK	980.15	Joback Method
cpg	859.16	J/molxK	1015.09	Joback Method
cpg	868.21	J/molxK	1050.03	Joback Method
cpg	876.23	J/molxK	1084.97	Joback Method
dvisc	0.0004290	Paxs	548.24	Joback Method

dvisc	0.0002609	Paxs	602.75	Joback Method
dvisc	0.0001723	Paxs	657.27	Joback Method
dvisc	0.0001212	Paxs	711.78	Joback Method
dvisc	0.0000897	Paxs	766.29	Joback Method
dvisc	0.0000691	Paxs	820.81	Joback Method
dvisc	0.0000549	Paxs	875.32	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406684&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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