

# Pimelic acid, 3,4-dichlorophenyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C17H22Cl2O4/c1-12(2)11-22-16(20)6-4-3-5-7-17(21)23-13-8-9-14(18)15(19)10
<b>InchiKey:</b>	DOMBJXNDWKLPAO-UHFFFAOYSA-N
<b>Formula:</b>	C17H22Cl2O4
<b>SMILES:</b>	CC(C)COC(=O)CCCCC(=O)Oc1ccc(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	361.26

## Physical Properties

Property code	Value	Unit	Source
gf	-308.73	kJ/mol	Joback Method
hf	-706.98	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	83.73	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.048		Crippen Method
mvol	265.990	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	852.00	K	Joback Method
tc	1063.90	K	Joback Method
tf	521.97	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.82	J/molxK	852.00	Joback Method
cpg	768.99	J/molxK	887.32	Joback Method
cpg	781.08	J/molxK	922.63	Joback Method
cpg	792.11	J/molxK	957.95	Joback Method
cpg	802.10	J/molxK	993.26	Joback Method
cpg	811.05	J/molxK	1028.58	Joback Method
cpg	818.99	J/molxK	1063.90	Joback Method
dvisc	0.0005217	Paxs	521.97	Joback Method

dvisc	0.0003039	Paxs	576.98	Joback Method
dvisc	0.0001945	Paxs	631.98	Joback Method
dvisc	0.0001337	Paxs	686.99	Joback Method
dvisc	0.0000971	Paxs	741.99	Joback Method
dvisc	0.0000738	Paxs	797.00	Joback Method
dvisc	0.0000580	Paxs	852.00	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416729&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416729&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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