

# Bis[4-(1,1-dimethylhexyl)phenyl] isophthalate

<b>Inchi:</b>	InChI=1S/C36H46O4/c1-7-9-11-24-35(3,4)29-16-20-31(21-17-29)39-33(37)27-14-13-15-
<b>InchiKey:</b>	IXLRPTGKJNYECCR-UHFFFAOYSA-N
<b>Formula:</b>	C36H46O4
<b>SMILES:</b>	CCCCC(C)(C)c1ccc(OC(=O)c2cccc(C(=O)Oc3ccc(C(C)(C)CCCC)cc3)c2)cc1
<b>Mol. weight [g/mol]:</b>	542.75

## Physical Properties

Property code	Value	Unit	Source
gf	98.42	kJ/mol	Joback Method
hf	-618.29	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	120.26	kJ/mol	Joback Method
log10ws	-11.62		Crippen Method
logp	9.841		Crippen Method
mvol	461.700	ml/mol	McGowan Method
pc	773.32	kPa	Joback Method
tb	1264.18	K	Joback Method
tc	1554.68	K	Joback Method
tf	761.46	K	Joback Method
vc	1.754	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1643.74	J/molxK	1264.18	Joback Method
cpg	1659.24	J/molxK	1312.60	Joback Method
cpg	1673.81	J/molxK	1361.01	Joback Method
cpg	1687.75	J/molxK	1409.43	Joback Method
cpg	1701.35	J/molxK	1457.85	Joback Method
cpg	1714.91	J/molxK	1506.26	Joback Method
cpg	1728.73	J/molxK	1554.68	Joback Method
dvisc	0.0000360	Paxs	761.46	Joback Method
dvisc	0.0000191	Paxs	845.25	Joback Method
dvisc	0.0000114	Paxs	929.03	Joback Method

dvisc	0.0000074	Paxs	1012.82	Joback Method
dvisc	0.0000051	Paxs	1096.61	Joback Method
dvisc	0.0000037	Paxs	1180.39	Joback Method
dvisc	0.0000028	Paxs	1264.18	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=B6004184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004184&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</a>

## Legend

<b>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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