

# Terephthalic acid, butyl 3-methylpentyl ester

<b>Inchi:</b>	InChI=1S/C18H26O4/c1-4-6-12-21-17(19)15-7-9-16(10-8-15)18(20)22-13-11-14(3)5-2/h
<b>InchiKey:</b>	LUBSJCNTDHSIBW-UHFFFAOYSA-N
<b>Formula:</b>	C18H26O4
<b>SMILES:</b>	CCCCOC(=O)c1ccc(C(=O)OCCC(C)CC)cc1
<b>Mol. weight [g/mol]:</b>	306.40

## Physical Properties

Property code	Value	Unit	Source
gf	-266.82	kJ/mol	Joback Method
hf	-684.67	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.237		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2250.00		NIST Webbook
tb	795.04	K	Joback Method
tc	997.07	K	Joback Method
tf	460.88	K	Joback Method
vc	0.978	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.78	J/molxK	795.04	Joback Method
cpg	777.64	J/molxK	828.71	Joback Method
cpg	792.42	J/molxK	862.38	Joback Method
cpg	806.14	J/molxK	896.06	Joback Method
cpg	818.82	J/molxK	929.73	Joback Method
cpg	830.46	J/molxK	963.40	Joback Method
cpg	841.10	J/molxK	997.07	Joback Method
dvisc	0.0008214	Paxs	460.88	Joback Method
dvisc	0.0004305	Paxs	516.57	Joback Method

dvisc	0.0002558	Paxs	572.27	Joback Method
dvisc	0.0001668	Paxs	627.96	Joback Method
dvisc	0.0001165	Paxs	683.65	Joback Method
dvisc	0.0000860	Paxs	739.35	Joback Method
dvisc	0.0000662	Paxs	795.04	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356674&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356674&amp;Units=SI</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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