

# Terephthalic acid, butyl 4-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C19H19NO6/c1-2-3-12-25-18(21)15-6-8-16(9-7-15)19(22)26-13-14-4-10-17(11
<b>InchiKey:</b>	ZTOUOOVGSJOTOL-UHFFFAOYSA-N
<b>Formula:</b>	C19H19NO6
<b>SMILES:</b>	CCCCOC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])cc2)cc1
<b>Mol. weight [g/mol]:</b>	357.36

## Physical Properties

Property code	Value	Unit	Source
gf	-117.63	kJ/mol	Joback Method
hf	-485.73	kJ/mol	Joback Method
hfus	49.20	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	3.909		Crippen Method
mvol	263.350	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
tb	1001.86	K	Joback Method
tc	1247.36	K	Joback Method
tf	669.70	K	Joback Method
vc	1.014	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.17	J/mol×K	1001.86	Joback Method
cpg	828.01	J/mol×K	1042.78	Joback Method
cpg	836.44	J/mol×K	1083.69	Joback Method
cpg	843.51	J/mol×K	1124.61	Joback Method
cpg	849.27	J/mol×K	1165.52	Joback Method
cpg	853.77	J/mol×K	1206.44	Joback Method
cpg	857.04	J/mol×K	1247.36	Joback Method

# Sources

<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=U416162&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416162&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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

Latest version available from:

<https://www.cheméo.com/cid/99-693-4/Terephthalic-acid-butyl-4-nitrobenzyl-ester.pdf>

Generated by Cheméo on 2024-04-25 14:39:03.300273989 +0000 UTC m=+16345192.220851300.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.