

# 4-Butylbenzoic acid, 8-chlorooctyl ester

<b>Inchi:</b>	InChI=1S/C19H29ClO2/c1-2-3-10-17-11-13-18(14-12-17)19(21)22-16-9-7-5-4-6-8-15-20
<b>InchiKey:</b>	DNIOWYNMKWZRSK-UHFFFAOYSA-N
<b>Formula:</b>	C19H29ClO2
<b>SMILES:</b>	CCCCc1ccc(C(=O)OCCCCCCCCCl)cc1
<b>Mol. weight [g/mol]:</b>	324.88

## Physical Properties

Property code	Value	Unit	Source
gf	-33.97	kJ/mol	Joback Method
hf	-470.97	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	74.37	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.765		Crippen Method
mvol	274.490	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	779.50	K	Joback Method
tc	975.71	K	Joback Method
tf	444.91	K	Joback Method
vc	1.065	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.77	J/molxK	779.50	Joback Method
cpg	815.62	J/molxK	812.20	Joback Method
cpg	831.45	J/molxK	844.90	Joback Method
cpg	846.30	J/molxK	877.61	Joback Method
cpg	860.21	J/molxK	910.31	Joback Method
cpg	873.21	J/molxK	943.01	Joback Method
cpg	885.33	J/molxK	975.71	Joback Method
dvisc	0.0009407	Paxs	444.91	Joback Method

dvisc	0.0004880	Paxs	500.68	Joback Method
dvisc	0.0002888	Paxs	556.44	Joback Method
dvisc	0.0001880	Paxs	612.20	Joback Method
dvisc	0.0001315	Paxs	667.97	Joback Method
dvisc	0.0000972	Paxs	723.73	Joback Method
dvisc	0.0000750	Paxs	779.50	Joback Method

## Sources

<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=U354322&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354322&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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