

# Butyric acid, 2-phenyl-, nonyl ester

<b>Inchi:</b>	InChI=1S/C19H30O2/c1-3-5-6-7-8-9-13-16-21-19(20)18(4-2)17-14-11-10-12-15-17/h10-1
<b>InchiKey:</b>	IZAZWQXMVONXHI-UHFFFAOYSA-N
<b>Formula:</b>	C19H30O2
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CC)c1ccccc1
<b>Mol. weight [g/mol]:</b>	290.44

## Physical Properties

Property code	Value	Unit	Source
gf	-14.85	kJ/mol	Joback Method
hf	-449.04	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.474		Crippen Method
mvol	262.250	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	736.65	K	Joback Method
tc	930.19	K	Joback Method
tf	387.47	K	Joback Method
vc	1.010	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.54	J/molxK	736.65	Joback Method
cpg	786.83	J/molxK	768.91	Joback Method
cpg	804.07	J/molxK	801.16	Joback Method
cpg	820.28	J/molxK	833.42	Joback Method
cpg	835.51	J/molxK	865.68	Joback Method
cpg	849.78	J/molxK	897.93	Joback Method
cpg	863.14	J/molxK	930.19	Joback Method
dvisc	0.0017401	Paxs	387.47	Joback Method

dvisc	0.0007395	Paxs	445.67	Joback Method
dvisc	0.0003830	Paxs	503.86	Joback Method
dvisc	0.0002273	Paxs	562.06	Joback Method
dvisc	0.0001488	Paxs	620.26	Joback Method
dvisc	0.0001047	Paxs	678.45	Joback Method
dvisc	0.0000779	Paxs	736.65	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=U406020&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406020&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</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>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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