

# Butyric acid, 2-phenyl-, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C23H22O3/c1-2-22(19-11-7-4-8-12-19)23(24)26-21-15-13-20(14-16-21)25-17-
InchiKey:	PIGCRLOQWZAHMD-UHFFFAOYSA-N
Formula:	C23H22O3
SMILES:	CCC(C(=O)O)c1ccc(OCc2ccccc2)cc1)c1ccccc1
Mol. weight [g/mol]:	346.42

## Physical Properties

Property code	Value	Unit	Source
gf	129.02	kJ/mol	Joback Method
hf	-202.23	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	85.46	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.365		Crippen Method
mvol	276.960	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	908.93	K	Joback Method
tc	1153.90	K	Joback Method
tf	520.14	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.17	J/molxK	908.93	Joback Method
cpg	857.87	J/molxK	949.76	Joback Method
cpg	871.04	J/molxK	990.59	Joback Method
cpg	882.74	J/molxK	1031.42	Joback Method
cpg	893.07	J/molxK	1072.24	Joback Method
cpg	902.10	J/molxK	1113.07	Joback Method
cpg	909.92	J/molxK	1153.90	Joback Method
dvisc	0.0004456	Paxs	520.14	Joback Method

dvisc	0.0002325	Paxs	584.94	Joback Method
dvisc	0.0001382	Paxs	649.74	Joback Method
dvisc	0.0000902	Paxs	714.54	Joback Method
dvisc	0.0000632	Paxs	779.33	Joback Method
dvisc	0.0000468	Paxs	844.13	Joback Method
dvisc	0.0000362	Paxs	908.93	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=U406877&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406877&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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