

# Butyric acid, 4-phenyl-, isobutyl ester

<b>Inchi:</b>	InChI=1S/C14H20O2/c1-12(2)11-16-14(15)10-6-9-13-7-4-3-5-8-13/h3-5,7-8,12H,6,9-11H
<b>InchiKey:</b>	YIDIILBHCSEKJF-UHFFFAOYSA-N
<b>Formula:</b>	C14H20O2
<b>SMILES:</b>	CC(C)COC(=O)CCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	220.31

## Physical Properties

Property code	Value	Unit	Source
gf	-56.95	kJ/mol	Joback Method
hf	-345.84	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	57.80	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.208		Crippen Method
mvol	191.800	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	622.25	K	Joback Method
tc	826.14	K	Joback Method
tf	331.12	K	Joback Method
vc	0.730	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.55	J/molxK	622.25	Joback Method
cpg	511.24	J/molxK	656.23	Joback Method
cpg	526.98	J/molxK	690.21	Joback Method
cpg	541.79	J/molxK	724.20	Joback Method
cpg	555.70	J/molxK	758.18	Joback Method
cpg	568.74	J/molxK	792.16	Joback Method
cpg	580.93	J/molxK	826.14	Joback Method
dvisc	0.0026271	Paxs	331.12	Joback Method

dvisc	0.0011824	Paxs	379.64	Joback Method
dvisc	0.0006378	Paxs	428.16	Joback Method
dvisc	0.0003900	Paxs	476.69	Joback Method
dvisc	0.0002612	Paxs	525.21	Joback Method
dvisc	0.0001872	Paxs	573.73	Joback Method
dvisc	0.0001414	Paxs	622.25	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=U406172&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406172&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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