

# Butyric acid, 4-phenyl-, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C24H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-16-22-26-24(25)21-17-20-23-18-14-13
<b>InchiKey:</b>	JSLHOTGAMVQVCD-UHFFFAOYSA-N
<b>Formula:</b>	C24H40O2
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	360.57

## Physical Properties

Property code	Value	Unit	Source
gf	29.69	kJ/mol	Joback Method
hf	-546.96	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.254		Crippen Method
mvol	332.700	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	851.49	K	Joback Method
tc	1046.47	K	Joback Method
tf	458.82	K	Joback Method
vc	1.296	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.64	J/molxK	851.49	Joback Method
cpg	1086.92	J/molxK	883.99	Joback Method
cpg	1105.03	J/molxK	916.48	Joback Method
cpg	1122.01	J/molxK	948.98	Joback Method
cpg	1137.91	J/molxK	981.47	Joback Method
cpg	1152.77	J/molxK	1013.97	Joback Method
cpg	1166.66	J/molxK	1046.47	Joback Method
dvisc	0.0008470	Paxs	458.82	Joback Method

dvisc	0.0003773	Paxs	524.26	Joback Method
dvisc	0.0002011	Paxs	589.71	Joback Method
dvisc	0.0001216	Paxs	655.15	Joback Method
dvisc	0.0000805	Paxs	720.60	Joback Method
dvisc	0.0000571	Paxs	786.04	Joback Method
dvisc	0.0000427	Paxs	851.49	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.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>
<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=U406184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406184&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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