

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

<b>Inchi:</b>	InChI=1S/C16H15NO4/c1-2-15(12-6-4-3-5-7-12)16(18)21-14-10-8-13(9-11-14)17(19)20/
<b>InchiKey:</b>	COAYZKDYHOUBLT-UHFFFAOYSA-N
<b>Formula:</b>	C16H15NO4
<b>SMILES:</b>	CCC(C(=O)Oc1ccc([N+](=O)[O-])cc1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	285.29

## Physical Properties

Property code	Value	Unit	Source
gf	98.22	kJ/mol	Joback Method
hf	-172.82	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.694		Crippen Method
mvol	213.640	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
tb	851.51	K	Joback Method
tc	1106.83	K	Joback Method
tf	536.21	K	Joback Method
vc	0.816	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.64	J/mol×K	851.51	Joback Method
cpg	632.50	J/mol×K	894.06	Joback Method
cpg	644.05	J/mol×K	936.62	Joback Method
cpg	654.36	J/mol×K	979.17	Joback Method
cpg	663.51	J/mol×K	1021.72	Joback Method
cpg	671.56	J/mol×K	1064.27	Joback Method
cpg	678.60	J/mol×K	1106.83	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=U406875&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406875&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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