

# Butyric acid, 4-nitrophenyl ester

<b>Inchi:</b>	InChI=1S/C10H11NO4/c1-2-3-10(12)15-9-6-4-8(5-7-9)11(13)14/h4-7H,2-3H2,1H3
<b>InchiKey:</b>	DVDUMIQZEUTAGK-UHFFFAOYSA-N
<b>Formula:</b>	C10H11NO4
<b>SMILES:</b>	CCCC(=O)Oc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	209.20
<b>CAS:</b>	2635-84-9

## Physical Properties

Property code	Value	Unit	Source
gf	-62.27	kJ/mol	Joback Method
hf	-280.23	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.300		Crippen Method
mvol	152.860	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	687.99	K	Joback Method
tc	925.31	K	Joback Method
tf	457.17	K	Joback Method
vc	0.594	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.14	J/mol×K	687.99	Joback Method
cpg	407.29	J/mol×K	727.54	Joback Method
cpg	418.53	J/mol×K	767.10	Joback Method
cpg	428.88	J/mol×K	806.65	Joback Method
cpg	438.36	J/mol×K	846.20	Joback Method
cpg	446.99	J/mol×K	885.75	Joback Method
cpg	454.81	J/mol×K	925.31	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=C2635849&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2635849&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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