

# Glutaric acid, butyl 3-nitrophenyl ester

<b>Inchi:</b>	InChI=1S/C15H19NO6/c1-2-3-10-21-14(17)8-5-9-15(18)22-13-7-4-6-12(11-13)16(19)20/
<b>InchiKey:</b>	JNEDIVJLRBYBBI-UHFFFAOYSA-N
<b>Formula:</b>	C15H19NO6
<b>SMILES:</b>	CCCCOC(=O)CCCC(=O)Oc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	309.31

## Physical Properties

Property code	Value	Unit	Source
gf	-254.09	kJ/mol	Joback Method
hf	-628.23	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	86.82	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.014		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpola	2439.00		NIST Webbook
tb	878.68	K	Joback Method
tc	1102.32	K	Joback Method
tf	585.68	K	Joback Method
vc	0.897	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.25	J/molxK	878.68	Joback Method
cpg	710.17	J/molxK	915.95	Joback Method
cpg	720.95	J/molxK	953.23	Joback Method
cpg	730.61	J/molxK	990.50	Joback Method
cpg	739.17	J/molxK	1027.77	Joback Method
cpg	746.64	J/molxK	1065.04	Joback Method
cpg	753.04	J/molxK	1102.32	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=U358889&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358889&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.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>

# 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>h vap:</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>m cvol:</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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