

# Glutaric acid, 2-ethylhexyl 2-nitrophenyl ester

<b>Inchi:</b>	InChI=1S/C19H27NO6/c1-3-5-9-15(4-2)14-25-18(21)12-8-13-19(22)26-17-11-7-6-10-16(
<b>InchiKey:</b>	MZRLJKYHDXJVIU-UHFFFAOYSA-N
<b>Formula:</b>	C19H27NO6
<b>SMILES:</b>	CCCCC(CC)COC(=O)CCCC(=O)Oc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	365.42

## Physical Properties

Property code	Value	Unit	Source
gf	-222.85	kJ/mol	Joback Method
hf	-716.07	kJ/mol	Joback Method
hfus	52.03	kJ/mol	Joback Method
hvap	95.34	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.430		Crippen Method
mvol	287.110	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	969.76	K	Joback Method
tc	1194.84	K	Joback Method
tf	615.76	K	Joback Method
vc	1.115	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.61	J/molxK	969.76	Joback Method
cpg	942.12	J/molxK	1007.27	Joback Method
cpg	953.29	J/molxK	1044.79	Joback Method
cpg	963.17	J/molxK	1082.30	Joback Method
cpg	971.79	J/molxK	1119.81	Joback Method
cpg	979.18	J/molxK	1157.33	Joback Method
cpg	985.37	J/molxK	1194.84	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=U393318&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393318&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>
<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>hvp:</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>rlnol:</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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