

# Glutaric acid, 3-methoxy-4-nitrobenzyl ethyl ester

Inchi:	InChI=1S/C15H19NO7/c1-3-22-14(17)5-4-6-15(18)23-10-11-7-8-12(16(19)20)13(9-11)21
InchiKey:	RPSPBPZWTNEDPN-UHFFFAOYSA-N
Formula:	C15H19NO7
SMILES:	CCOC(=O)CCCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
Mol. weight [g/mol]:	325.31

## Physical Properties

Property code	Value	Unit	Source
gf	-368.72	kJ/mol	Joback Method
hf	-771.92	kJ/mol	Joback Method
hfus	45.99	kJ/mol	Joback Method
hvap	89.90	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.380		Crippen Method
mcvol	236.620	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinqol	2550.00		NIST Webbook
tb	906.08	K	Joback Method
tc	1129.95	K	Joback Method
tf	620.43	K	Joback Method
vc	0.915	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.65	J/molxK	906.08	Joback Method
cpg	733.82	J/molxK	943.39	Joback Method
cpg	743.73	J/molxK	980.70	Joback Method
cpg	752.37	J/molxK	1018.02	Joback Method
cpg	759.74	J/molxK	1055.33	Joback Method
cpg	765.82	J/molxK	1092.64	Joback Method
cpg	770.63	J/molxK	1129.95	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=U376889&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376889&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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