

# Glutaric acid, monoamide, N-(3-methylphenyl)-, butyl ester

Inchi:	InChI=1S/C16H23NO3/c1-3-4-11-20-16(19)10-6-9-15(18)17-14-8-5-7-13(2)12-14/h5,7-8,
InchiKey:	YMYHJKPNNNOJGM-UHFFFAOYSA-N
Formula:	C16H23NO3
SMILES:	CCCCOC(=O)CCCC(=O)Nc1cccc(C)c1
Mol. weight [g/mol]:	277.36

## Physical Properties

Property code	Value	Unit	Source
gf	-86.83	kJ/mol	Joback Method
hf	-452.42	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.447		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpola	2592.00		NIST Webbook
rinpola	2592.00		NIST Webbook
tb	777.47	K	Joback Method
tc	981.54	K	Joback Method
tf	483.77	K	Joback Method
vc	0.888	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.89	J/molxK	777.47	Joback Method
cpg	691.69	J/molxK	811.48	Joback Method
cpg	705.50	J/molxK	845.49	Joback Method
cpg	718.36	J/molxK	879.50	Joback Method
cpg	730.30	J/molxK	913.51	Joback Method
cpg	741.33	J/molxK	947.53	Joback Method
cpg	751.49	J/molxK	981.54	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360915&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360915&amp;Units=SI</a>
<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>

# 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>rinp:</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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