

# Glutaric acid, monoamide, N-(4-ethylphenyl)-, ethyl ester

<b>Inchi:</b>	InChI=1S/C15H21NO3/c1-3-12-8-10-13(11-9-12)16-14(17)6-5-7-15(18)19-4-2/h8-11H,3-
<b>InchiKey:</b>	CAYFWSOQODAHNN-UHFFFAOYSA-N
<b>Formula:</b>	C15H21NO3
<b>SMILES:</b>	CCOC(=O)CCCC(=O)Nc1ccc(CC)cc1
<b>Mol. weight [g/mol]:</b>	263.33

## Physical Properties

Property code	Value	Unit	Source
gf	-95.25	kJ/mol	Joback Method
hf	-431.78	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.921		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpola	2522.00		NIST Webbook
tb	754.59	K	Joback Method
tc	960.29	K	Joback Method
tf	472.50	K	Joback Method
vc	0.833	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.45	J/mol×K	754.59	Joback Method
cpg	635.94	J/mol×K	788.87	Joback Method
cpg	649.47	J/mol×K	823.16	Joback Method
cpg	662.07	J/mol×K	857.44	Joback Method
cpg	673.77	J/mol×K	891.72	Joback Method
cpg	684.59	J/mol×K	926.01	Joback Method
cpg	694.55	J/mol×K	960.29	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360895&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>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>mccvol:</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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