

# Glutaric acid, 2,3-dimethylphenyl ethyl ester

<b>Inchi:</b>	InChI=1S/C15H20O4/c1-4-18-14(16)9-6-10-15(17)19-13-8-5-7-11(2)12(13)3/h5,7-8H,4,6
<b>InchiKey:</b>	UEARIBZUGRQGBX-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O4
<b>SMILES:</b>	CCOC(=O)CCCC(=O)Oc1cccc(C)c1C
<b>Mol. weight [g/mol]:</b>	264.32

## Physical Properties

Property code	Value	Unit	Source
gf	-299.27	kJ/mol	Joback Method
hf	-628.94	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.942		Crippen Method
mvol	213.330	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	731.82	K	Joback Method
tc	936.25	K	Joback Method
tf	454.59	K	Joback Method
vc	0.816	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.78	J/molxK	731.82	Joback Method
cpg	656.98	J/molxK	902.18	Joback Method
cpg	645.96	J/molxK	868.11	Joback Method
cpg	634.03	J/molxK	834.04	Joback Method
cpg	621.19	J/molxK	799.96	Joback Method
cpg	607.44	J/molxK	765.89	Joback Method
cpg	667.10	J/molxK	936.25	Joback Method
dvisc	0.0001058	Paxs	731.82	Joback Method

dvisc	0.0001319	Paxs	685.62	Joback Method
dvisc	0.0001697	Paxs	639.41	Joback Method
dvisc	0.0002270	Paxs	593.21	Joback Method
dvisc	0.0003191	Paxs	547.00	Joback Method
dvisc	0.0004776	Paxs	500.80	Joback Method
dvisc	0.0007757	Paxs	454.59	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359295&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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