

# Glutaric acid, (2-methylcyclohex-1-enyl)methyl 2-ethylhexyl

Inchi:  
ester

InChI=1S/C21H36O4/c1-4-6-11-18(5-2)15-24-20(22)13-9-14-21(23)25-16-19-12-8-7-10-

InchiKey:

MDLWGYAKHFTHRA-UHFFFAOYSA-N

Formula:

C21H36O4

SMILES:

CCCCC(CC)COC(=O)CCCC(=O)OCC1=C(C)CCCC1

Mol. weight [g/mol]:

352.51

## Physical Properties

Property code	Value	Unit	Source
gf	-301.48	kJ/mol	Joback Method
hf	-862.15	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.350		Crippen Method
mvol	306.470	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
tb	865.36	K	Joback Method
tc	1066.89	K	Joback Method
tf	493.17	K	Joback Method
vc	1.173	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.37	J/mol×K	865.36	Joback Method
cpg	1013.26	J/mol×K	898.95	Joback Method
cpg	1029.85	J/mol×K	932.54	Joback Method
cpg	1045.17	J/mol×K	966.12	Joback Method
cpg	1059.23	J/mol×K	999.71	Joback Method
cpg	1072.07	J/mol×K	1033.30	Joback Method
cpg	1083.71	J/mol×K	1066.89	Joback Method
dvisc	0.0006258	Paxs	493.17	Joback Method

dvisc	0.0003006	Paxs	555.20	Joback Method
dvisc	0.0001674	Paxs	617.23	Joback Method
dvisc	0.0001037	Paxs	679.26	Joback Method
dvisc	0.0000696	Paxs	741.30	Joback Method
dvisc	0.0000497	Paxs	803.33	Joback Method
dvisc	0.0000372	Paxs	865.36	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405506&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405506&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>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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