

# Glutaric acid, 3-ethylphenyl hexadecyl ester

<b>Inchi:</b>	InChI=1S/C29H48O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-24-32-28(30)22-19-23-29
<b>InchiKey:</b>	SSOCMQCUHMFRLS-UHFFFAOYSA-N
<b>Formula:</b>	C29H48O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(CC)c1
<b>Mol. weight [g/mol]:</b>	460.69

## Physical Properties

Property code	Value	Unit	Source
gf	-171.76	kJ/mol	Joback Method
hf	-906.43	kJ/mol	Joback Method
hfus	70.09	kJ/mol	Joback Method
hvap	101.40	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	8.349		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	774.18	kPa	Joback Method
rinpol	3454.00		NIST Webbook
rinpol	3454.00		NIST Webbook
tb	1047.16	K	Joback Method
tc	1291.10	K	Joback Method
tf	599.85	K	Joback Method
vc	1.599	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.07	J/molxK	1047.16	Joback Method
cpg	1507.75	J/molxK	1250.44	Joback Method
cpg	1496.34	J/molxK	1209.79	Joback Method
cpg	1483.25	J/molxK	1169.13	Joback Method
cpg	1468.40	J/molxK	1128.47	Joback Method
cpg	1451.70	J/molxK	1087.82	Joback Method
cpg	1517.56	J/molxK	1291.10	Joback Method
dvisc	0.0000143	Paxs	1047.16	Joback Method

dvisc	0.0000189	Paxs	972.61	Joback Method
dvisc	0.0000260	Paxs	898.06	Joback Method
dvisc	0.0000380	Paxs	823.50	Joback Method
dvisc	0.0000598	Paxs	748.95	Joback Method
dvisc	0.0001042	Paxs	674.40	Joback Method
dvisc	0.0002083	Paxs	599.85	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=U359172&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359172&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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