

# Glutaric acid, 2-ethylhexyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C26H34O5/c1-3-5-11-21(4-2)19-29-25(27)16-10-17-26(28)30-20-22-12-9-15-2
InchiKey:	PJYHRMMNGOOHRG-UHFFFAOYSA-N
Formula:	C26H34O5
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	426.55

## Physical Properties

Property code	Value	Unit	Source
gf	-192.05	kJ/mol	Joback Method
hf	-745.48	kJ/mol	Joback Method
hfus	54.03	kJ/mol	Joback Method
hvap	99.02	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.452		Crippen Method
mvol	350.430	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	3136.00		NIST Webbook
rinpol	3136.00		NIST Webbook
tb	1027.18	K	Joback Method
tc	1258.50	K	Joback Method
tf	599.69	K	Joback Method
vc	1.335	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.20	J/molxK	1027.18	Joback Method
cpg	1216.11	J/molxK	1219.94	Joback Method
cpg	1209.10	J/molxK	1181.39	Joback Method
cpg	1200.56	J/molxK	1142.84	Joback Method
cpg	1190.43	J/molxK	1104.29	Joback Method
cpg	1178.66	J/molxK	1065.73	Joback Method
cpg	1221.62	J/molxK	1258.50	Joback Method
dvisc	0.0000158	Paxs	1027.18	Joback Method

dvisc	0.0000206	Paxs	955.93	Joback Method
dvisc	0.0000281	Paxs	884.68	Joback Method
dvisc	0.0000404	Paxs	813.43	Joback Method
dvisc	0.0000624	Paxs	742.19	Joback Method
dvisc	0.0001054	Paxs	670.94	Joback Method
dvisc	0.0002020	Paxs	599.69	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=U392129&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392129&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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