

# Glutaric acid, octyl 3-phenylpropyl ester

<b>Inchi:</b>	InChI=1S/C22H34O4/c1-2-3-4-5-6-10-18-25-21(23)16-11-17-22(24)26-19-12-15-20-13-8
<b>InchiKey:</b>	NSNSACUGZAXBOA-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	362.50

## Physical Properties

Property code	Value	Unit	Source
gf	-221.07	kJ/mol	Joback Method
hf	-750.48	kJ/mol	Joback Method
hfus	52.35	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.236		Crippen Method
mvol	311.960	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rmpol	2750.00		NIST Webbook
tb	882.02	K	Joback Method
tc	1084.27	K	Joback Method
tf	508.44	K	Joback Method
vc	1.208	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.85	J/molxK	882.02	Joback Method
cpg	1014.49	J/molxK	915.73	Joback Method
cpg	1029.92	J/molxK	949.44	Joback Method
cpg	1044.16	J/molxK	983.15	Joback Method
cpg	1057.25	J/molxK	1016.86	Joback Method
cpg	1069.21	J/molxK	1050.57	Joback Method
cpg	1080.10	J/molxK	1084.27	Joback Method
dvisc	0.0005610	Paxs	508.44	Joback Method
dvisc	0.0002853	Paxs	570.70	Joback Method

dvisc	0.0001657	Paxs	632.97	Joback Method
dvisc	0.0001061	Paxs	695.23	Joback Method
dvisc	0.0000731	Paxs	757.49	Joback Method
dvisc	0.0000533	Paxs	819.76	Joback Method
dvisc	0.0000406	Paxs	882.02	Joback Method

## Sources

<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=U360137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360137&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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