

# Glutaric acid, 2,6-dimethoxyphenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C19H28O6/c1-4-5-6-7-14-24-17(20)12-9-13-18(21)25-19-15(22-2)10-8-11-16(
<b>InchiKey:</b>	WXXPTBVCJKIIIQ-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O6
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC
<b>Mol. weight [g/mol]:</b>	352.42

## Physical Properties

Property code	Value	Unit	Source
gf	-475.59	kJ/mol	Joback Method
hf	-975.94	kJ/mol	Joback Method
hfus	46.18	kJ/mol	Joback Method
hvap	84.62	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.903		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinqol	2604.00		NIST Webbook
tb	868.18	K	Joback Method
tc	1070.93	K	Joback Method
tf	544.13	K	Joback Method
vc	1.075	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.26	J/molxK	868.18	Joback Method
cpg	891.10	J/molxK	901.97	Joback Method
cpg	904.68	J/molxK	935.76	Joback Method
cpg	917.00	J/molxK	969.56	Joback Method
cpg	928.02	J/molxK	1003.35	Joback Method
cpg	937.76	J/molxK	1037.14	Joback Method
cpg	946.19	J/molxK	1070.93	Joback Method
dvisc	0.0002841	Paxs	544.13	Joback Method
dvisc	0.0001723	Paxs	598.14	Joback Method

dvisc	0.0001136	Paxs	652.15	Joback Method
dvisc	0.0000798	Paxs	706.15	Joback Method
dvisc	0.0000589	Paxs	760.16	Joback Method
dvisc	0.0000453	Paxs	814.17	Joback Method
dvisc	0.0000360	Paxs	868.18	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U358709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358709&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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