

# Glutaric acid, 3-methylbut-2-en-1-yl 2-propylphenyl ester

<b>Inchi:</b>	InChI=1S/C19H26O4/c1-4-8-16-9-5-6-10-17(16)23-19(21)12-7-11-18(20)22-14-13-15(2)3
<b>InchiKey:</b>	VCUNESWXODGMRC-UHFFFAOYSA-N
<b>Formula:</b>	C19H26O4
<b>SMILES:</b>	CCCc1ccccc1OC(=O)CCCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	318.41

## Physical Properties

Property code	Value	Unit	Source
gf	-184.29	kJ/mol	Joback Method
hf	-592.60	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.224		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpola	2265.00		NIST Webbook
tb	822.40	K	Joback Method
tc	1028.52	K	Joback Method
tf	468.11	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.70	J/mol×K	822.40	Joback Method
cpg	808.27	J/mol×K	856.75	Joback Method
cpg	822.78	J/mol×K	891.11	Joback Method
cpg	836.27	J/mol×K	925.46	Joback Method
cpg	848.77	J/mol×K	959.82	Joback Method
cpg	860.31	J/mol×K	994.17	Joback Method
cpg	870.92	J/mol×K	1028.52	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=U392140&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392140&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>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>mccvol:</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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