

# Diglycolic acid, butyl 2-isopropylphenyl ester

<b>Inchi:</b>	InChI=1S/C17H24O5/c1-4-5-10-21-16(18)11-20-12-17(19)22-15-9-7-6-8-14(15)13(2)3/h6
<b>InchiKey:</b>	XQAFHZNVEBXBAN-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O5
<b>SMILES:</b>	CCCCOC(=O)COCC(=O)Oc1ccccc1C(C)C
<b>Mol. weight [g/mol]:</b>	308.37

## Physical Properties

Property code	Value	Unit	Source
gf	-380.24	kJ/mol	Joback Method
hf	-796.25	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.075		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2572.00		NIST Webbook
rinpol	2572.00		NIST Webbook
tb	794.58	K	Joback Method
tc	997.23	K	Joback Method
tf	471.84	K	Joback Method
vc	0.940	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.23	J/molxK	794.58	Joback Method
cpg	748.43	J/molxK	828.36	Joback Method
cpg	762.53	J/molxK	862.13	Joback Method
cpg	775.55	J/molxK	895.91	Joback Method
cpg	787.49	J/molxK	929.68	Joback Method
cpg	798.35	J/molxK	963.46	Joback Method
cpg	808.13	J/molxK	997.23	Joback Method
dvisc	0.0006330	Paxs	471.84	Joback Method

dvisc	0.0003456	Paxs	525.63	Joback Method
dvisc	0.0002112	Paxs	579.42	Joback Method
dvisc	0.0001403	Paxs	633.21	Joback Method
dvisc	0.0000994	Paxs	687.00	Joback Method
dvisc	0.0000740	Paxs	740.79	Joback Method
dvisc	0.0000573	Paxs	794.58	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=U382288&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382288&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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