

# Diglycolic acid, 2-isopropylphenyl octyl ester

<b>Inchi:</b>	InChI=1S/C21H32O5/c1-4-5-6-7-8-11-14-25-20(22)15-24-16-21(23)26-19-13-10-9-12-18
<b>InchiKey:</b>	VMZAPLIQYJQNC-UHFFFAOYSA-N
<b>Formula:</b>	C21H32O5
<b>SMILES:</b>	CCCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)C
<b>Mol. weight [g/mol]:</b>	364.48

## Physical Properties

Property code	Value	Unit	Source
gf	-346.56	kJ/mol	Joback Method
hf	-878.81	kJ/mol	Joback Method
hfus	47.04	kJ/mol	Joback Method
hvap	85.61	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.636		Crippen Method
mvol	303.740	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	886.10	K	Joback Method
tc	1090.63	K	Joback Method
tf	516.92	K	Joback Method
vc	1.163	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.23	J/molxK	886.10	Joback Method
cpg	1033.79	J/molxK	1056.54	Joback Method
cpg	1023.03	J/molxK	1022.46	Joback Method
cpg	1011.00	J/molxK	988.37	Joback Method
cpg	997.70	J/molxK	954.28	Joback Method
cpg	983.12	J/molxK	920.19	Joback Method
cpg	1043.30	J/molxK	1090.63	Joback Method
dvisc	0.0000325	Paxs	886.10	Joback Method

dvisc	0.0000425	Paxs	824.57	Joback Method
dvisc	0.0000579	Paxs	763.04	Joback Method
dvisc	0.0000833	Paxs	701.51	Joback Method
dvisc	0.0001286	Paxs	639.98	Joback Method
dvisc	0.0002177	Paxs	578.45	Joback Method
dvisc	0.0004176	Paxs	516.92	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382293&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382293&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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