

# Diglycolic acid, ethyl 2-naphthyl ester

<b>Inchi:</b>	InChI=1S/C16H16O5/c1-2-20-15(17)10-19-11-16(18)21-14-8-7-12-5-3-4-6-13(12)9-14/h3
<b>InchiKey:</b>	PDKPYOMMXCQONF-UHFFFAOYSA-N
<b>Formula:</b>	C16H16O5
<b>SMILES:</b>	CCOC(=O)COCC(=O)Oc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	288.30

## Physical Properties

Property code	Value	Unit	Source
gf	-279.57	kJ/mol	Joback Method
hf	-579.26	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	76.51	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.325		Crippen Method
mvol	213.830	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rmpol	2896.00		NIST Webbook
rmpol	2896.00		NIST Webbook
tb	791.12	K	Joback Method
tc	1010.91	K	Joback Method
tf	508.27	K	Joback Method
vc	0.811	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.97	J/molxK	791.12	Joback Method
cpg	660.16	J/molxK	974.28	Joback Method
cpg	651.08	J/molxK	937.65	Joback Method
cpg	641.05	J/molxK	901.02	Joback Method
cpg	630.03	J/molxK	864.38	Joback Method
cpg	618.01	J/molxK	827.75	Joback Method
cpg	668.30	J/molxK	1010.91	Joback Method
dvisc	0.0001355	Paxs	791.12	Joback Method

dvisc	0.0001637	Paxs	743.98	Joback Method
dvisc	0.0002029	Paxs	696.84	Joback Method
dvisc	0.0002594	Paxs	649.70	Joback Method
dvisc	0.0003447	Paxs	602.55	Joback Method
dvisc	0.0004806	Paxs	555.41	Joback Method
dvisc	0.0007128	Paxs	508.27	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381786&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381786&amp;Units=SI</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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