

# Diglycolic acid, hexyl 2-naphthyl ester

<b>Inchi:</b>	InChI=1S/C20H24O5/c1-2-3-4-7-12-24-19(21)14-23-15-20(22)25-18-11-10-16-8-5-6-9-17
<b>InchiKey:</b>	KLWDSDKSHRWINW-UHFFFAOYSA-N
<b>Formula:</b>	C20H24O5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)Oc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	344.40

## Physical Properties

Property code	Value	Unit	Source
gf	-245.89	kJ/mol	Joback Method
hf	-661.82	kJ/mol	Joback Method
hfus	44.99	kJ/mol	Joback Method
hvap	85.41	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.885		Crippen Method
mvol	270.190	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	3384.00		NIST Webbook
rinpol	3384.00		NIST Webbook
tb	882.64	K	Joback Method
tc	1096.67	K	Joback Method
tf	553.35	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.62	J/molxK	882.64	Joback Method
cpg	889.41	J/molxK	1061.00	Joback Method
cpg	879.79	J/molxK	1025.33	Joback Method
cpg	869.14	J/molxK	989.65	Joback Method
cpg	857.42	J/molxK	953.98	Joback Method
cpg	844.59	J/molxK	918.31	Joback Method
cpg	898.02	J/molxK	1096.67	Joback Method
dvisc	0.0000821	Paxs	882.64	Joback Method

dvisc	0.0001009	Paxs	827.76	Joback Method
dvisc	0.0001275	Paxs	772.88	Joback Method
dvisc	0.0001672	Paxs	718.00	Joback Method
dvisc	0.0002292	Paxs	663.11	Joback Method
dvisc	0.0003326	Paxs	608.23	Joback Method
dvisc	0.0005198	Paxs	553.35	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=U381790&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381790&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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