

# Diglycolic acid, hexadecyl propyl ester

<b>Inchi:</b>	InChI=1S/C23H44O5/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19-28-23(25)21-26-20-22
<b>InchiKey:</b>	VDAUBQBXBIZDTO-UHFFFAOYSA-N
<b>Formula:</b>	C23H44O5
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	400.59

## Physical Properties

Property code	Value	Unit	Source
gf	-430.06	kJ/mol	Joback Method
hf	-1139.87	kJ/mol	Joback Method
hfus	62.09	kJ/mol	Joback Method
hvap	87.51	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.981		Crippen Method
mvol	355.680	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	3472.00		NIST Webbook
rinpol	3472.00		NIST Webbook
tb	900.64	K	Joback Method
tc	1103.95	K	Joback Method
tf	515.52	K	Joback Method
vc	1.389	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.66	J/molxK	900.64	Joback Method
cpg	1269.34	J/molxK	1070.07	Joback Method
cpg	1255.63	J/molxK	1036.18	Joback Method
cpg	1240.53	J/molxK	1002.30	Joback Method
cpg	1224.02	J/molxK	968.41	Joback Method
cpg	1206.06	J/molxK	934.53	Joback Method
cpg	1281.67	J/molxK	1103.95	Joback Method
dvisc	0.0000253	Paxs	900.64	Joback Method

dvisc	0.0000337	Paxs	836.45	Joback Method
dvisc	0.0000469	Paxs	772.27	Joback Method
dvisc	0.0000693	Paxs	708.08	Joback Method
dvisc	0.0001109	Paxs	643.89	Joback Method
dvisc	0.0001968	Paxs	579.71	Joback Method
dvisc	0.0004027	Paxs	515.52	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.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>
<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=U381852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381852&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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