

# Diglycolic acid, heptyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C15H28O5/c1-4-5-6-7-8-9-19-14(16)11-18-12-15(17)20-10-13(2)3/h13H,4-12H
<b>InchiKey:</b>	RVPGHDLXAKPFAV-UHFFFAOYSA-N
<b>Formula:</b>	C15H28O5
<b>SMILES:</b>	CCCCCCCOC(=O)COCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	288.38

## Physical Properties

Property code	Value	Unit	Source
gf	-499.86	kJ/mol	Joback Method
hf	-980.03	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.716		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinsol	2336.00		NIST Webbook
rinsol	2336.00		NIST Webbook
tb	717.16	K	Joback Method
tc	895.78	K	Joback Method
tf	410.36	K	Joback Method
vc	0.935	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.24	J/molxK	717.16	Joback Method
cpg	723.36	J/molxK	746.93	Joback Method
cpg	738.68	J/molxK	776.70	Joback Method
cpg	753.17	J/molxK	806.47	Joback Method
cpg	766.84	J/molxK	836.24	Joback Method
cpg	779.69	J/molxK	866.01	Joback Method
cpg	791.71	J/molxK	895.78	Joback Method
dvisc	0.0011434	Paxs	410.36	Joback Method

dvisc	0.0005637	Paxs	461.49	Joback Method
dvisc	0.0003200	Paxs	512.63	Joback Method
dvisc	0.0002013	Paxs	563.76	Joback Method
dvisc	0.0001368	Paxs	614.89	Joback Method
dvisc	0.0000986	Paxs	666.03	Joback Method
dvisc	0.0000745	Paxs	717.16	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382130&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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