

# Diglycolic acid, 4-bromophenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C16H21BrO5/c1-2-3-4-5-10-21-15(18)11-20-12-16(19)22-14-8-6-13(17)7-9-14
<b>InchiKey:</b>	MFSSEUUJKJODRN-UHFFFAOYSA-N
<b>Formula:</b>	C16H21BrO5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	373.24

## Physical Properties

Property code	Value	Unit	Source
gf	-371.90	kJ/mol	Joback Method
hf	-744.00	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	81.31	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.495		Crippen Method
mvol	250.790	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
tb	838.30	K	Joback Method
tc	1049.74	K	Joback Method
tf	535.37	K	Joback Method
vc	0.952	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.55	J/molxK	838.30	Joback Method
cpg	769.35	J/molxK	1014.50	Joback Method
cpg	760.49	J/molxK	979.26	Joback Method
cpg	750.59	J/molxK	944.02	Joback Method
cpg	739.64	J/molxK	908.78	Joback Method
cpg	727.63	J/molxK	873.54	Joback Method
cpg	777.17	J/molxK	1049.74	Joback Method
dvisc	0.0000576	Paxs	838.30	Joback Method

dvisc	0.0000722	Paxs	787.81	Joback Method
dvisc	0.0000932	Paxs	737.32	Joback Method
dvisc	0.0001250	Paxs	686.84	Joback Method
dvisc	0.0001756	Paxs	636.35	Joback Method
dvisc	0.0002615	Paxs	585.86	Joback Method
dvisc	0.0004199	Paxs	535.37	Joback Method

## Sources

<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=U381898&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381898&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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