

# Diglycolic acid, 4-bromophenyl propyl ester

<b>Inchi:</b>	InChI=1S/C13H15BrO5/c1-2-7-18-12(15)8-17-9-13(16)19-11-5-3-10(14)4-6-11/h3-6H,2,7
<b>InchiKey:</b>	WOGSWIVLFVNZHO-UHFFFAOYSA-N
<b>Formula:</b>	C13H15BrO5
<b>SMILES:</b>	CCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	331.16

## Physical Properties

Property code	Value	Unit	Source
gf	-397.16	kJ/mol	Joback Method
hf	-682.08	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	74.63	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.324		Crippen Method
mvol	208.520	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	769.66	K	Joback Method
tc	986.67	K	Joback Method
tf	501.56	K	Joback Method
vc	0.783	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.77	J/molxK	769.66	Joback Method
cpg	601.11	J/molxK	950.50	Joback Method
cpg	592.72	J/molxK	914.33	Joback Method
cpg	583.39	J/molxK	878.17	Joback Method
cpg	573.12	J/molxK	842.00	Joback Method
cpg	561.91	J/molxK	805.83	Joback Method
cpg	608.55	J/molxK	986.67	Joback Method
dvisc	0.0000880	Paxs	769.66	Joback Method

dvisc	0.0001089	Paxs	724.98	Joback Method
dvisc	0.0001386	Paxs	680.29	Joback Method
dvisc	0.0001824	Paxs	635.61	Joback Method
dvisc	0.0002503	Paxs	590.93	Joback Method
dvisc	0.0003617	Paxs	546.24	Joback Method
dvisc	0.0005582	Paxs	501.56	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=U381893&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381893&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>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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