

# Succinic acid, 3-bromobenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C14H17BrO4/c1-2-8-18-13(16)6-7-14(17)19-10-11-4-3-5-12(15)9-11/h3-5,9H,2
<b>InchiKey:</b>	DHLPDFNKUSGHCZ-UHFFFAOYSA-N
<b>Formula:</b>	C14H17BrO4
<b>SMILES:</b>	CCCOC(=O)CCC(=O)OCc1cccc(Br)c1
<b>Mol. weight [g/mol]:</b>	329.19

## Physical Properties

Property code	Value	Unit	Source
gf	-283.74	kJ/mol	Joback Method
hf	-570.50	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.226		Crippen Method
mvol	216.740	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	770.12	K	Joback Method
tc	986.25	K	Joback Method
tf	490.60	K	Joback Method
vc	0.822	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.72	J/molxK	770.12	Joback Method
cpg	590.59	J/molxK	806.14	Joback Method
cpg	602.53	J/molxK	842.16	Joback Method
cpg	613.53	J/molxK	878.18	Joback Method
cpg	623.64	J/molxK	914.21	Joback Method
cpg	632.85	J/molxK	950.23	Joback Method
cpg	641.19	J/molxK	986.25	Joback Method
dvisc	0.0007115	Paxs	490.60	Joback Method

dvisc	0.0004468	Paxs	537.19	Joback Method
dvisc	0.0003022	Paxs	583.77	Joback Method
dvisc	0.0002166	Paxs	630.36	Joback Method
dvisc	0.0001625	Paxs	676.95	Joback Method
dvisc	0.0001265	Paxs	723.53	Joback Method
dvisc	0.0001015	Paxs	770.12	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=U382413&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382413&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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