

# Succinic acid, 4-bromophenethyl isobutyl ester

Inchi:	InChI=1S/C16H21BrO4/c1-12(2)11-21-16(19)8-7-15(18)20-10-9-13-3-5-14(17)6-4-13/h3
InchiKey:	LSORMESADRYXSA-UHFFFAOYSA-N
Formula:	C16H21BrO4
SMILES:	CC(C)COC(=O)CCC(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	357.24

## Physical Properties

Property code	Value	Unit	Source
gf	-269.34	kJ/mol	Joback Method
hf	-617.06	kJ/mol	Joback Method
hfus	38.18	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.514		Crippen Method
mvol	244.920	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	815.44	K	Joback Method
tc	1030.25	K	Joback Method
tf	498.14	K	Joback Method
vc	0.927	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.18	J/molxK	815.44	Joback Method
cpg	701.88	J/molxK	851.24	Joback Method
cpg	714.53	J/molxK	887.04	Joback Method
cpg	726.16	J/molxK	922.85	Joback Method
cpg	736.79	J/molxK	958.65	Joback Method
cpg	746.45	J/molxK	994.45	Joback Method
cpg	755.17	J/molxK	1030.25	Joback Method
dvisc	0.0006585	Paxs	498.14	Joback Method

dvisc	0.0003796	Paxs	551.02	Joback Method
dvisc	0.0002410	Paxs	603.91	Joback Method
dvisc	0.0001647	Paxs	656.79	Joback Method
dvisc	0.0001191	Paxs	709.67	Joback Method
dvisc	0.0000900	Paxs	762.56	Joback Method
dvisc	0.0000706	Paxs	815.44	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381432&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381432&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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