

# Succinic acid, 7-bromoheptyl butyl ester

**Inchi:** InChI=1S/C15H27BrO4/c1-2-3-12-19-14(17)9-10-15(18)20-13-8-6-4-5-7-11-16/h2-13H2,  
**InchiKey:** MQYCDKRGPGXBKE-UHFFFAOYSA-N  
**Formula:** C15H27BrO4  
**SMILES:** CCCOC(=O)CCC(=O)OCCCCCBr  
**Mol. weight [g/mol]:** 351.28

## Physical Properties

Property code	Value	Unit	Source
gf	-378.10	kJ/mol	Joback Method
hf	-816.20	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.998		Crippen Method
mvol	254.590	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	761.34	K	Joback Method
tc	948.45	K	Joback Method
tf	462.93	K	Joback Method
vc	0.986	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.51	J/molxK	761.34	Joback Method
cpg	790.04	J/molxK	917.27	Joback Method
cpg	778.35	J/molxK	886.08	Joback Method
cpg	765.86	J/molxK	854.90	Joback Method
cpg	752.57	J/molxK	823.71	Joback Method
cpg	738.46	J/molxK	792.53	Joback Method
cpg	800.95	J/molxK	948.45	Joback Method
dvisc	0.0000867	Paxs	761.34	Joback Method

dvisc	0.0001115	Paxs	711.61	Joback Method
dvisc	0.0001490	Paxs	661.87	Joback Method
dvisc	0.0002087	Paxs	612.13	Joback Method
dvisc	0.0003103	Paxs	562.40	Joback Method
dvisc	0.0004981	Paxs	512.66	Joback Method
dvisc	0.0008853	Paxs	462.93	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=U382405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382405&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>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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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