

# Phthalic acid, 7-bromoheptyl octyl ester

<b>Inchi:</b>	InChI=1S/C23H35BrO4/c1-2-3-4-5-8-13-18-27-22(25)20-15-10-11-16-21(20)23(26)28-19
<b>InchiKey:</b>	LOZPOSNYPNOTIJ-UHFFFAOYSA-N
<b>Formula:</b>	C23H35BrO4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCBr
<b>Mol. weight [g/mol]:</b>	455.43

## Physical Properties

Property code	Value	Unit	Source
gf	-207.96	kJ/mol	Joback Method
hf	-756.26	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	6.706		Crippen Method
mvol	343.550	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	976.04	K	Joback Method
tc	1195.50	K	Joback Method
tf	592.03	K	Joback Method
vc	1.325	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.41	J/molxK	976.04	Joback Method
cpg	1113.53	J/molxK	1012.62	Joback Method
cpg	1127.34	J/molxK	1049.19	Joback Method
cpg	1139.90	J/molxK	1085.77	Joback Method
cpg	1151.24	J/molxK	1122.35	Joback Method
cpg	1161.43	J/molxK	1158.93	Joback Method
cpg	1170.51	J/molxK	1195.50	Joback Method
dvisc	0.0002740	Paxs	592.03	Joback Method

dvisc	0.0001544	Paxs	656.03	Joback Method
dvisc	0.0000964	Paxs	720.03	Joback Method
dvisc	0.0000650	Paxs	784.03	Joback Method
dvisc	0.0000465	Paxs	848.04	Joback Method
dvisc	0.0000348	Paxs	912.04	Joback Method
dvisc	0.0000271	Paxs	976.04	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=U415522&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415522&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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