

# Phthalic acid, 8-bromooctyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C20H29BrO4/c1-16(2)15-25-20(23)18-12-8-7-11-17(18)19(22)24-14-10-6-4-3-5
<b>InchiKey:</b>	TWQRUGRSPOYCMV-UHFFFAOYSA-N
<b>Formula:</b>	C20H29BrO4
<b>SMILES:</b>	CC(C)COC(=O)c1cccc1C(=O)OCCCCCCCCBr
<b>Mol. weight [g/mol]:</b>	413.35

## Physical Properties

Property code	Value	Unit	Source
gf	-235.66	kJ/mol	Joback Method
hf	-699.62	kJ/mol	Joback Method
hfus	48.54	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.392		Crippen Method
mvol	301.280	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	3102.00		NIST Webbook
rinpol	3102.00		NIST Webbook
tb	906.96	K	Joback Method
tc	1119.93	K	Joback Method
tf	543.22	K	Joback Method
vc	1.151	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.65	J/molxK	906.96	Joback Method
cpg	979.85	J/molxK	1084.44	Joback Method
cpg	969.82	J/molxK	1048.94	Joback Method
cpg	958.72	J/molxK	1013.45	Joback Method
cpg	946.52	J/molxK	977.95	Joback Method
cpg	933.17	J/molxK	942.46	Joback Method
cpg	988.85	J/molxK	1119.93	Joback Method
dvisc	0.0000392	Paxs	906.96	Joback Method

dvisc	0.0000506	Paxs	846.34	Joback Method
dvisc	0.0000680	Paxs	785.71	Joback Method
dvisc	0.0000959	Paxs	725.09	Joback Method
dvisc	0.0001441	Paxs	664.47	Joback Method
dvisc	0.0002349	Paxs	603.84	Joback Method
dvisc	0.0004271	Paxs	543.22	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382553&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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