

# Phthalic acid, 7-bromoheptyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C19H27BrO4/c1-15(2)14-24-19(22)17-11-7-6-10-16(17)18(21)23-13-9-5-3-4-8
<b>InchiKey:</b>	KKFDWYKZRSDENJ-UHFFFAOYSA-N
<b>Formula:</b>	C19H27BrO4
<b>SMILES:</b>	CC(C)COC(=O)c1cccc1C(=O)OCCCCCBr
<b>Mol. weight [g/mol]:</b>	399.32

## Physical Properties

Property code	Value	Unit	Source
gf	-244.08	kJ/mol	Joback Method
hf	-678.98	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.002		Crippen Method
mvol	287.190	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2769.00		NIST Webbook
rinpol	2769.00		NIST Webbook
tb	884.08	K	Joback Method
tc	1096.44	K	Joback Method
tf	531.95	K	Joback Method
vc	1.095	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.87	J/molxK	884.08	Joback Method
cpg	874.21	J/molxK	919.47	Joback Method
cpg	887.40	J/molxK	954.87	Joback Method
cpg	899.50	J/molxK	990.26	Joback Method
cpg	910.52	J/molxK	1025.65	Joback Method
cpg	920.50	J/molxK	1061.04	Joback Method
cpg	929.47	J/molxK	1096.44	Joback Method
dvisc	0.0004785	Paxs	531.95	Joback Method

dvisc	0.0002661	Paxs	590.64	Joback Method
dvisc	0.0001646	Paxs	649.33	Joback Method
dvisc	0.0001102	Paxs	708.01	Joback Method
dvisc	0.0000785	Paxs	766.70	Joback Method
dvisc	0.0000586	Paxs	825.39	Joback Method
dvisc	0.0000456	Paxs	884.08	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415517&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415517&amp;Units=SI</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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