

# Phthalic acid, 2-(2-bromophenyl)ethyl butyl ester

Inchi:	InChI=1S/C20H21BrO4/c1-2-3-13-24-19(22)16-9-5-6-10-17(16)20(23)25-14-12-15-8-4-7
InchiKey:	NDLJLWCOTWJAHP-UHFFFAOYSA-N
Formula:	C20H21BrO4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1Br
Mol. weight [g/mol]:	405.28

## Physical Properties

Property code	Value	Unit	Source
gf	-130.44	kJ/mol	Joback Method
hf	-469.28	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.806		Crippen Method
mcvol	277.520	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinsol	2664.00		NIST Webbook
tb	939.06	K	Joback Method
tc	1173.28	K	Joback Method
tf	597.16	K	Joback Method
vc	1.050	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.72	J/molxK	939.06	Joback Method
cpg	825.86	J/molxK	978.10	Joback Method
cpg	836.75	J/molxK	1017.13	Joback Method
cpg	846.44	J/molxK	1056.17	Joback Method
cpg	854.98	J/molxK	1095.21	Joback Method
cpg	862.41	J/molxK	1134.24	Joback Method
cpg	868.78	J/molxK	1173.28	Joback Method
dvisc	0.0003142	Paxs	597.16	Joback Method
dvisc	0.0001976	Paxs	654.14	Joback Method

dvisc	0.0001339	Paxs	711.13	Joback Method
dvisc	0.0000961	Paxs	768.11	Joback Method
dvisc	0.0000722	Paxs	825.09	Joback Method
dvisc	0.0000563	Paxs	882.08	Joback Method
dvisc	0.0000452	Paxs	939.06	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=U377759&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377759&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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