

# Isophthalic acid, 4-bromophenyl nonyl ester

<b>Inchi:</b>	InChI=1S/C23H27BrO4/c1-2-3-4-5-6-7-8-16-27-22(25)18-10-9-11-19(17-18)23(26)28-21
<b>InchiKey:</b>	KRRMVCPENVVIPF-UHFFFAOYSA-N
<b>Formula:</b>	C23H27BrO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
<b>Mol. weight [g/mol]:</b>	447.36

## Physical Properties

Property code	Value	Unit	Source
gf	-105.18	kJ/mol	Joback Method
hf	-531.20	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	97.42	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	6.576		Crippen Method
mvol	319.790	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
tb	1007.70	K	Joback Method
tc	1241.48	K	Joback Method
tf	630.97	K	Joback Method
vc	1.218	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.51	J/molxK	1007.70	Joback Method
cpg	1001.91	J/molxK	1046.66	Joback Method
cpg	1013.00	J/molxK	1085.63	Joback Method
cpg	1022.83	J/molxK	1124.59	Joback Method
cpg	1031.46	J/molxK	1163.55	Joback Method
cpg	1038.96	J/molxK	1202.51	Joback Method
cpg	1045.39	J/molxK	1241.48	Joback Method
dvisc	0.0002246	Paxs	630.97	Joback Method

dvisc	0.0001367	Paxs	693.76	Joback Method
dvisc	0.0000903	Paxs	756.55	Joback Method
dvisc	0.0000636	Paxs	819.34	Joback Method
dvisc	0.0000471	Paxs	882.12	Joback Method
dvisc	0.0000363	Paxs	944.91	Joback Method
dvisc	0.0000289	Paxs	1007.70	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=U344472&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344472&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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