

# Isophthalic acid, 4-bromophenyl isoheptyl ester

Inchi:	InChI=1S/C20H21BrO4/c1-14(2)5-4-12-24-19(22)15-6-3-7-16(13-15)20(23)25-18-10-8-1
InchiKey:	LKZZXQMLYABCDB-UHFFFAOYSA-N
Formula:	C20H21BrO4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
Mol. weight [g/mol]:	405.28

## Physical Properties

Property code	Value	Unit	Source
gf	-132.88	kJ/mol	Joback Method
hf	-474.56	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.261		Crippen Method
mvol	277.520	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	938.62	K	Joback Method
tc	1175.56	K	Joback Method
tf	582.16	K	Joback Method
vc	1.044	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.22	J/molxK	938.62	Joback Method
cpg	826.45	J/molxK	978.11	Joback Method
cpg	837.38	J/molxK	1017.60	Joback Method
cpg	847.07	J/molxK	1057.09	Joback Method
cpg	855.56	J/molxK	1096.58	Joback Method
cpg	862.91	J/molxK	1136.07	Joback Method
cpg	869.16	J/molxK	1175.56	Joback Method
dvisc	0.0003364	Paxs	582.16	Joback Method

dvisc	0.0002017	Paxs	641.57	Joback Method
dvisc	0.0001318	Paxs	700.98	Joback Method
dvisc	0.0000921	Paxs	760.39	Joback Method
dvisc	0.0000678	Paxs	819.80	Joback Method
dvisc	0.0000520	Paxs	879.21	Joback Method
dvisc	0.0000412	Paxs	938.62	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=U344468&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344468&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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