

# Phthalic acid, 2-(4-bromophenyl)ethyl dodecyl ester

Inchi:	InChI=1S/C28H37BrO4/c1-2-3-4-5-6-7-8-9-10-13-21-32-27(30)25-14-11-12-15-26(25)28
InchiKey:	XESLYEVFEAHDIV-UHFFFAOYSA-N
Formula:	C28H37BrO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	517.50

## Physical Properties

Property code	Value	Unit	Source
gf	-63.08	kJ/mol	Joback Method
hf	-634.40	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	108.55	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	7.926		Crippen Method
mvol	390.240	ml/mol	McGowan Method
pc	1031.91	kPa	Joback Method
rinpol	3604.00		NIST Webbook
rinpol	3604.00		NIST Webbook
tb	1122.10	K	Joback Method
tc	1374.66	K	Joback Method
tf	687.32	K	Joback Method
vc	1.498	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.28	J/molxK	1122.10	Joback Method
cpg	1305.27	J/molxK	1164.19	Joback Method
cpg	1316.72	J/molxK	1206.29	Joback Method
cpg	1326.71	J/molxK	1248.38	Joback Method
cpg	1335.37	J/molxK	1290.47	Joback Method
cpg	1342.77	J/molxK	1332.56	Joback Method
cpg	1349.04	J/molxK	1374.66	Joback Method
dvisc	0.0001215	Paxs	687.32	Joback Method

dvisc	0.0000704	Paxs	759.78	Joback Method
dvisc	0.0000449	Paxs	832.25	Joback Method
dvisc	0.0000307	Paxs	904.71	Joback Method
dvisc	0.0000223	Paxs	977.17	Joback Method
dvisc	0.0000169	Paxs	1049.64	Joback Method
dvisc	0.0000132	Paxs	1122.10	Joback Method

## Sources

<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=U378045&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378045&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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