

Phthalic acid, 2-(4-bromophenyl)ethyl undecyl ester

Inchi:	InChI=1S/C27H35BrO4/c1-2-3-4-5-6-7-8-9-12-20-31-26(29)24-13-10-11-14-25(24)27(30)
InchiKey:	JYNFZWHEOFIHCL-UHFFFAOYSA-N
Formula:	C27H35BrO4
SMILES:	CCCCCCCCCOC(=O)c1cccc1C(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	503.47

Physical Properties

Property code	Value	Unit	Source
gf	-71.50	kJ/mol	Joback Method
hf	-613.76	kJ/mol	Joback Method
hfus	63.85	kJ/mol	Joback Method
hvap	106.32	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	7.536		Crippen Method
mvol	376.150	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	3505.00		NIST Webbook
rinpol	3505.00		NIST Webbook
tb	1099.22	K	Joback Method
tc	1345.78	K	Joback Method
tf	676.05	K	Joback Method
vc	1.442	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.93	J/molxK	1099.22	Joback Method
cpg	1243.77	J/molxK	1140.31	Joback Method
cpg	1255.12	J/molxK	1181.41	Joback Method
cpg	1265.07	J/molxK	1222.50	Joback Method
cpg	1273.71	J/molxK	1263.59	Joback Method
cpg	1281.14	J/molxK	1304.69	Joback Method
cpg	1287.44	J/molxK	1345.78	Joback Method
dvisc	0.0001381	Paxs	676.05	Joback Method

dvisc	0.0000808	Paxs	746.58	Joback Method
dvisc	0.0000518	Paxs	817.11	Joback Method
dvisc	0.0000357	Paxs	887.63	Joback Method
dvisc	0.0000259	Paxs	958.16	Joback Method
dvisc	0.0000197	Paxs	1028.69	Joback Method
dvisc	0.0000155	Paxs	1099.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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