Phthalic acid, 2-(3-bromophenyl)ethyl undecyl ester

Inchi: InChI=1S/C27H35BrO4/c1-2-3-4-5-6-7-8-9-12-19-31-26(29)24-16-10-11-17-25(24)27(30)
InchiKey: XAPZDPAQBOLZBM-UHFFFAOYSA-N
Formula: C27H35BrO4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1
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
mcvol	376.150	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	3485.00		NIST Webbook
rinpol	3485.00		NIST Webbook
tb	1099.22	K	Joback Method
tc	1345.78	K	Joback Method
tf	676.05	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.93	J/mol×K	1099.22	Joback Method
cpg	1281.14	J/mol×K	1304.69	Joback Method
cpg	1273.71	J/mol×K	1263.59	Joback Method
cpg	1265.07	J/mol×K	1222.50	Joback Method
cpg	1255.12	J/mol×K	1181.41	Joback Method
cpg	1243.77	J/mol×K	1140.31	Joback Method
cpg	1287.44	J/mol×K	1345.78	Joback Method
dvisc	0.0000155	Pa×s	1099.22	Joback Method

dvisc	0.0000197	Pa×s	1028.69	Joback Method
dvisc	0.0000259	Pa×s	958.16	Joback Method
dvisc	0.0000357	Pa×s	887.63	Joback Method
dvisc	0.0000518	Pa×s	817.11	Joback Method
dvisc	0.0000808	Pa×s	746.58	Joback Method
dvisc	0.0001381	Pa×s	676.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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