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

Inchi: InChI=1S/C27H35BrO5/c1-2-3-4-5-6-7-8-9-12-19-32-26(29)24-13-10-11-14-25(24)27(30)
InchiKey: ROJPDMHJWHQHSS-UHFFFAOYSA-N
Formula: C27H35BrO5
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 519.47

Physical Properties

Property code	Value	Unit	Source
gf	-176.50	kJ/mol	Joback Method
hf	-745.98	kJ/mol	Joback Method
hfus	65.04	kJ/mol	Joback Method
hvap	108.73	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	7.372		Crippen Method
mcvol	382.020	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	3533.00		NIST Webbook
rinpol	3533.00		NIST Webbook
tb	1121.64	K	Joback Method
tc	1373.94	K	Joback Method
tf	698.28	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.06	J/mol×K	1121.64	Joback Method
cpg	1294.18	J/mol×K	1331.89	Joback Method
cpg	1289.64	J/mol×K	1289.84	Joback Method
cpg	1283.53	J/mol×K	1247.79	Joback Method
cpg	1275.78	J/mol×K	1205.74	Joback Method
cpg	1266.31	J/mol×K	1163.69	Joback Method
cpg	1297.23	J/mol×K	1373.94	Joback Method
dvisc	0.0000113	Pa×s	1121.64	Joback Method

dvisc	0.0000143	Pa×s	1051.08	Joback Method
dvisc	0.0000188	Pa×s	980.52	Joback Method
dvisc	0.0000257	Pa×s	909.96	Joback Method
dvisc	0.0000371	Pa×s	839.40	Joback Method
dvisc	0.0000572	Pa×s	768.84	Joback Method
dvisc	0.0000963	Pa×s	698.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382900&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