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

Inchi: InChI=1S/C21H23BrO5/c1-2-3-6-13-26-20(23)18-7-4-5-8-19(18)21(24)27-15-14-25-17-11

InchiKey: AEXVOXYXZQBHIT-UHFFFAOYSA-N

Formula: C21H23BrO5

SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc(Br)cc1

Mol. weight [g/mol]: 435.31

Physical Properties

Property code	Value	Unit	Source
gf	-227.02	kJ/mol	Joback Method
hf	-622.14	kJ/mol	Joback Method
hfus	49.50	kJ/mol	Joback Method
hvap	95.37	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.032		Crippen Method
mcvol	297.480	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	984.36	K	Joback Method
tc	1217.89	K	Joback Method
tf	630.66	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.51	J/mol×K	984.36	Joback Method
cpg	908.79	J/mol×K	1023.28	Joback Method
cpg	918.65	J/mol×K	1062.20	Joback Method
cpg	927.13	J/mol×K	1101.13	Joback Method
cpg	934.26	J/mol×K	1140.05	Joback Method
cpg	940.08	J/mol×K	1178.97	Joback Method
cpg	944.61	J/mol×K	1217.89	Joback Method
dvisc	0.0001997	Pa×s	630.66	Joback Method

dvisc	0.0001260	Pa×s	689.61	Joback Method
dvisc	0.0000855	Pa×s	748.56	Joback Method
dvisc	0.0000614	Pa×s	807.51	Joback Method
dvisc	0.0000461	Pa×s	866.46	Joback Method
dvisc	0.0000359	Pa×s	925.41	Joback Method
dvisc	0.0000288	Pa×s	984.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382894&Units=SI

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