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

Inchi: InChI=1S/C22H25BrO5/c1-2-3-4-7-14-27-21(24)19-8-5-6-9-20(19)22(25)28-16-15-26-18-

InchiKey: DBKWDKWQERSXNJ-UHFFFAOYSA-N

Formula: C22H25BrO5

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

Mol. weight [g/mol]: 449.33

Physical Properties

Property code	Value	Unit	Source
gf	-218.60	kJ/mol	Joback Method
hf	-642.78	kJ/mol	Joback Method
hfus	52.09	kJ/mol	Joback Method
hvap	97.60	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.422		Crippen Method
mcvol	311.570	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	3032.00		NIST Webbook
rinpol	3032.00		NIST Webbook
tb	1007.24	K	Joback Method
tc	1241.38	K	Joback Method
tf	641.93	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.06	J/mol×K	1007.24	Joback Method
cpg	967.35	J/mol×K	1046.26	Joback Method
cpg	977.18	J/mol×K	1085.29	Joback Method
cpg	985.59	J/mol×K	1124.31	Joback Method
cpg	992.62	J/mol×K	1163.33	Joback Method
cpg	998.31	J/mol×K	1202.35	Joback Method
cpg	1002.68	J/mol×K	1241.38	Joback Method
dvisc	0.0001780	Pa×s	641.93	Joback Method

dvisc	0.0001111	Pa×s	702.82	Joback Method
dvisc	0.0000748	Pa×s	763.70	Joback Method
dvisc	0.0000534	Pa×s	824.59	Joback Method
dvisc	0.0000399	Pa×s	885.47	Joback Method
dvisc	0.0000310	Pa×s	946.36	Joback Method
dvisc	0.0000248	Pa×s	1007.24	Joback Method

Sources

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=U382895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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