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

Inchi: InChI=1S/C20H21BrO5/c1-14(2)13-26-20(23)18-6-4-3-5-17(18)19(22)25-12-11-24-16-9-7

InchiKey: XTADTZSFBFCOQI-UHFFFAOYSA-N

Formula: C20H21BrO5

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCCOc1ccc(Br)cc1

Mol. weight [g/mol]: 421.28

Physical Properties

Property code	Value	Unit	Source
gf	-237.88	kJ/mol	Joback Method
hf	-606.78	kJ/mol	Joback Method
hfus	43.38	kJ/mol	Joback Method
hvap	92.76	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.498		Crippen Method
mcvol	283.390	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	961.04	K	Joback Method
tc	1197.23	K	Joback Method
tf	604.39	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.96	J/mol×K	961.04	Joback Method
cpg	882.57	J/mol×K	1157.87	Joback Method
cpg	876.78	J/mol×K	1118.50	Joback Method
cpg	869.65	J/mol×K	1079.14	Joback Method
cpg	861.16	J/mol×K	1039.77	Joback Method
cpg	851.27	J/mol×K	1000.41	Joback Method
cpg	887.05	J/mol×K	1197.23	Joback Method
dvisc	0.0000306	Pa×s	961.04	Joback Method

dvisc	0.0000384	Pa×s	901.60	Joback Method
dvisc	0.0000499	Pa×s	842.16	Joback Method
dvisc	0.0000674	Pa×s	782.72	Joback Method
dvisc	0.0000957	Pa×s	723.27	Joback Method
dvisc	0.0001448	Pa×s	663.83	Joback Method
dvisc	0.0002374	Pa×s	604.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382892&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