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

Inchi: InChI=1S/C20H21BrO5/c1-2-3-12-25-19(22)17-6-4-5-7-18(17)20(23)26-14-13-24-16-10-8

InchiKey: YULIMMDZAKYTNL-UHFFFAOYSA-N

Formula: C20H21BrO5

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

Mol. weight [g/mol]: 421.28

Physical Properties

Property code	Value	Unit	Source
gf	-235.44	kJ/mol	Joback Method
hf	-601.50	kJ/mol	Joback Method
hfus	46.91	kJ/mol	Joback Method
hvap	93.15	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.642		Crippen Method
mcvol	283.390	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2832.00		NIST Webbook
rinpol	2832.00		NIST Webbook
tb	961.48	K	Joback Method
tc	1195.28	K	Joback Method
tf	619.39	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.49	J/mol×K	961.48	Joback Method
cpg	882.25	J/mol×K	1156.31	Joback Method
cpg	876.35	J/mol×K	1117.35	Joback Method
cpg	869.15	J/mol×K	1078.38	Joback Method
cpg	860.62	J/mol×K	1039.41	Joback Method
cpg	850.75	J/mol×K	1000.45	Joback Method
cpg	886.89	J/mol×K	1195.28	Joback Method
dvisc	0.0000335	Pa×s	961.48	Joback Method

dvisc	0.0000416	Pa×s	904.47	Joback Method
dvisc	0.0000532	Pa×s	847.45	Joback Method
dvisc	0.0000705	Pa×s	790.43	Joback Method
dvisc	0.0000975	Pa×s	733.42	Joback Method
dvisc	0.0001425	Pa×s	676.40	Joback Method
dvisc	0.0002234	Pa×s	619.39	Joback Method

Sources

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=U382893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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