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

Inchi: InChI=1S/C25H31BrO5/c1-2-3-4-5-6-7-10-17-30-24(27)22-11-8-9-12-23(22)25(28)31-19-
InchiKey: MZHFXCRPIWGTMO-UHFFFAOYSA-N
Formula: C25H31BrO5
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 491.42

Physical Properties

Property code	Value	Unit	Source
gf	-193.34	kJ/mol	Joback Method
hf	-704.70	kJ/mol	Joback Method
hfus	59.86	kJ/mol	Joback Method
hvap	104.28	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	6.592		Crippen Method
mcvol	353.840	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	3335.00		NIST Webbook
rinpol	3335.00		NIST Webbook
tb	1075.88	K	Joback Method
tc	1317.64	K	Joback Method
tf	675.74	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.39	J/mol×K	1075.88	Joback Method
cpg	1175.04	J/mol×K	1277.35	Joback Method
cpg	1169.93	J/mol×K	1237.05	Joback Method
cpg	1163.37	J/mol×K	1196.76	Joback Method
cpg	1155.30	J/mol×K	1156.47	Joback Method
cpg	1145.66	J/mol×K	1116.17	Joback Method
cpg	1178.73	J/mol×K	1317.64	Joback Method
dvisc	0.0000155	Pa×s	1075.88	Joback Method

dvisc	0.0000196	Pa×s	1009.19	Joback Method
dvisc	0.0000255	Pa×s	942.50	Joback Method
dvisc	0.0000346	Pa×s	875.81	Joback Method
dvisc	0.0000494	Pa×s	809.12	Joback Method
dvisc	0.0000751	Pa×s	742.43	Joback Method
dvisc	0.0001240	Pa×s	675.74	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=U382898&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