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

Inchi: InChI=1S/C23H27BrO5/c1-2-3-4-5-8-15-28-22(25)20-9-6-7-10-21(20)23(26)29-17-16-27-
InchiKey: SMNPUFHCQOHCRU-UHFFFAOYSA-N
Formula: C23H27BrO5
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 463.36

Physical Properties

Property code	Value	Unit	Source
gf	-210.18	kJ/mol	Joback Method
hf	-663.42	kJ/mol	Joback Method
hfus	54.68	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.812		Crippen Method
mcvol	325.660	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	3133.00		NIST Webbook
rinpol	3133.00		NIST Webbook
tb	1030.12	K	Joback Method
tc	1265.79	K	Joback Method
tf	653.20	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.09	J/mol×K	1030.12	Joback Method
cpg	1026.37	J/mol×K	1069.40	Joback Method
cpg	1036.15	J/mol×K	1108.68	Joback Method
cpg	1044.47	J/mol×K	1147.96	Joback Method
cpg	1051.37	J/mol×K	1187.24	Joback Method
cpg	1056.90	J/mol×K	1226.51	Joback Method
cpg	1061.09	J/mol×K	1265.79	Joback Method
dvisc	0.0001582	Pa×s	653.20	Joback Method

dvisc	0.0000977	Pa×s	716.02	Joback Method
dvisc	0.0000653	Pa×s	778.84	Joback Method
dvisc	0.0000463	Pa×s	841.66	Joback Method
dvisc	0.0000344	Pa×s	904.48	Joback Method
dvisc	0.0000266	Pa×s	967.30	Joback Method
dvisc	0.0000212	Pa×s	1030.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382896&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

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