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

Inchi: InChI=1S/C24H29BrO5/c1-2-3-4-5-6-9-16-29-23(26)21-10-7-8-11-22(21)24(27)30-18-17-

InchiKey: YPLVDBAOUYHZPC-UHFFFAOYSA-N

Formula: C24H29BrO5

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

Mol. weight [g/mol]: 477.39

Physical Properties

Property code	Value	Unit	Source
gf	-201.76	kJ/mol	Joback Method
hf	-684.06	kJ/mol	Joback Method
hfus	57.27	kJ/mol	Joback Method
hvap	102.05	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.202		Crippen Method
mcvol	339.750	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	3236.00		NIST Webbook
rinpol	3236.00		NIST Webbook
tb	1053.00	K	Joback Method
tc	1291.19	K	Joback Method
tf	664.47	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.55	J/mol×K	1053.00	Joback Method
cpg	1085.82	J/mol×K	1092.70	Joback Method
cpg	1095.54	J/mol×K	1132.40	Joback Method
cpg	1103.75	J/mol×K	1172.10	Joback Method
cpg	1110.49	J/mol×K	1211.80	Joback Method
cpg	1115.82	J/mol×K	1251.49	Joback Method
cpg	1119.79	J/mol×K	1291.19	Joback Method
dvisc	0.0001402	Pa×s	664.47	Joback Method

dvisc	0.0000858	Pa×s	729.23	Joback Method
dvisc	0.0000568	Pa×s	793.98	Joback Method
dvisc	0.0000401	Pa×s	858.74	Joback Method
dvisc	0.0000297	Pa×s	923.49	Joback Method
dvisc	0.0000229	Pa×s	988.25	Joback Method
dvisc	0.0000182	Pa×s	1053.00	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=U382897&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