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

Inchi: InChI=1S/C28H37BrO5/c1-2-3-4-5-6-7-8-9-10-13-20-33-27(30)25-14-11-12-15-26(25)28(

InchiKey: XHRICMNZBULCOR-UHFFFAOYSA-N

Formula: C28H37BrO5

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

Mol. weight [g/mol]: 533.49

Physical Properties

Property code	Value	Unit	Source
gf	-168.08	kJ/mol	Joback Method
hf	-766.62	kJ/mol	Joback Method
hfus	67.63	kJ/mol	Joback Method
hvap	110.95	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	7.763		Crippen Method
mcvol	396.110	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	3632.00		NIST Webbook
rinpol	3632.00		NIST Webbook
tb	1144.52	K	Joback Method
tc	1403.94	K	Joback Method
tf	709.55	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.81	J/mol×K	1144.52	Joback Method
cpg	1354.04	J/mol×K	1360.70	Joback Method
cpg	1349.84	J/mol×K	1317.46	Joback Method
cpg	1344.00	J/mol×K	1274.23	Joback Method
cpg	1336.44	J/mol×K	1230.99	Joback Method
cpg	1327.07	J/mol×K	1187.76	Joback Method
cpg	1356.70	J/mol×K	1403.94	Joback Method
dvisc	0.0000096	Pa×s	1144.52	Joback Method

dvisc	0.0000122	Pa×s	1072.03	Joback Method
dvisc	0.0000161	Pa×s	999.53	Joback Method
dvisc	0.0000221	Pa×s	927.04	Joback Method
dvisc	0.0000321	Pa×s	854.54	Joback Method
dvisc	0.0000498	Pa×s	782.05	Joback Method
dvisc	0.0000846	Pa×s	709.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382901&Units=SI

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