Phthalic acid, 2-(3-bromophenyl)ethyl dodecyl ester

Inchi: InChI=1S/C28H37BrO4/c1-2-3-4-5-6-7-8-9-10-13-20-32-27(30)25-17-11-12-18-26(25)28(

InchiKey: CREXTQDOYKVFSI-UHFFFAOYSA-N

Formula: C28H37BrO4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 517.50

Physical Properties

Property code	Value	Unit	Source
gf	-63.08	kJ/mol	Joback Method
hf	-634.40	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	108.55	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	7.926		Crippen Method
mcvol	390.240	ml/mol	McGowan Method
pc	1031.91	kPa	Joback Method
rinpol	3585.00		NIST Webbook
tb	1122.10	K	Joback Method
tc	1374.66	K	Joback Method
tf	687.32	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.28	J/mol×K	1122.10	Joback Method
cpg	1305.27	J/mol×K	1164.19	Joback Method
cpg	1316.72	J/mol×K	1206.29	Joback Method
cpg	1326.71	J/mol×K	1248.38	Joback Method
cpg	1335.37	J/mol×K	1290.47	Joback Method
cpg	1342.77	J/mol×K	1332.56	Joback Method
cpg	1349.04	J/mol×K	1374.66	Joback Method
dvisc	0.0001215	Pa×s	687.32	Joback Method
dvisc	0.0000704	Pa×s	759.78	Joback Method

dvisc	0.0000449	Pa×s	832.25	Joback Method
dvisc	0.0000307	Pa×s	904.71	Joback Method
dvisc	0.0000223	Pa×s	977.17	Joback Method
dvisc	0.0000169	Pa×s	1049.64	Joback Method
dvisc	0.0000132	Pa×s	1122.10	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=U378031&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