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

Inchi: InChI=1S/C29H39BrO4/c1-2-3-4-5-6-7-8-9-10-11-14-21-33-28(31)26-18-12-13-19-27(26)
InchiKey: VBGACYVPYJTPCZ-UHFFFAOYSA-N
Formula: C29H39BrO4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]: 531.52

Physical Properties

Property code	Value	Unit	Source
gf	-54.66	kJ/mol	Joback Method
hf	-655.04	kJ/mol	Joback Method
hfus	69.03	kJ/mol	Joback Method
hvap	110.77	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.316		Crippen Method
mcvol	404.330	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
rinpol	3687.00		NIST Webbook
rinpol	3687.00		NIST Webbook
tb	1144.98	K	Joback Method
tc	1404.80	K	Joback Method
tf	698.59	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.95	J/mol×K	1144.98	Joback Method
cpg	1367.14	J/mol×K	1188.28	Joback Method
cpg	1378.70	J/mol×K	1231.59	Joback Method
cpg	1388.76	J/mol×K	1274.89	Joback Method
cpg	1397.43	J/mol×K	1318.19	Joback Method
cpg	1404.82	J/mol×K	1361.49	Joback Method
cpg	1411.07	J/mol×K	1404.80	Joback Method
dvisc	0.0001067	Pa×s	698.59	Joback Method

dvisc	0.0000613	Pa×s	772.99	Joback Method
dvisc	0.0000388	Pa×s	847.39	Joback Method
dvisc	0.0000264	Pa×s	921.79	Joback Method
dvisc	0.0000191	Pa×s	996.18	Joback Method
dvisc	0.0000144	Pa×s	1070.58	Joback Method
dvisc	0.0000113	Pa×s	1144.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378032&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