Benzoic acid, 4,4'-(tetramethyl-1,3-cyclobutanediylidenedinitrilo diethyl ester

Inchi: InChI=1S/C26H30N2O4/c1-7-31-21(29)17-9-13-19(14-10-17)27-23-25(3,4)24(26(23,5)6)
InchiKey: JAPXVCXRUBQQQL-UHFFFAOYSA-N
Formula: C26H30N2O4
SMILES: CCOC(=O)c1ccc(N=C2C(C)(C)C(=Nc3ccc(C(=O)OCC)cc3)C2(C)C)cc1
Mol. weight [g/mol]: 434.53
CAS: 1690-30-8

Physical Properties

Property code	Value	Unit	Source
hf	-460.61	kJ/mol	Joback Method
hvap	103.42	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.951		Crippen Method
mcvol	345.060	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
tb	1175.32	K	Joback Method
tc	1441.70	K	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=C1690308&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature