

3,3',5,5'-Tetratert-butyl-2'-(propionyloxy)[1,1'-biphenyl]-2-carboxylate propionate

InChI: InChI=1S/C34H50O4/c1-15-27(35)37-29-23(17-21(31(3,4)5)19-25(29)33(9,10)11)24-18-7
InChIKey: RUOVIWYDPBGTRX-UHFFFAOYSA-N

Formula: C34H50O4

SMILES: CCC(=O)Oc1c(-c2cc(C(C)(C)C)cc(C(C)(C)C)c2OC(=O)CC)cc(C(C)(C)C)cc1C(C)(C)C

Mol. weight [g/mol]: 522.76

Physical Properties

Property code	Value	Unit	Source
gf	-54.04	kJ/mol	Joback Method
hf	-865.45	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	112.93	kJ/mol	Joback Method
log10ws	-10.79		Crippen Method
logp	9.174		Crippen Method
mcvol	457.280	ml/mol	McGowan Method
pc	714.15	kPa	Joback Method
tb	1200.22	K	Joback Method
tc	1471.78	K	Joback Method
tf	754.90	K	Joback Method
vc	1.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.27	J/mol×K	1200.22	Joback Method
cpg	1720.70	J/mol×K	1426.52	Joback Method
cpg	1704.55	J/mol×K	1381.26	Joback Method
cpg	1688.29	J/mol×K	1336.00	Joback Method
cpg	1671.66	J/mol×K	1290.74	Joback Method
cpg	1654.40	J/mol×K	1245.48	Joback Method
cpg	1736.98	J/mol×K	1471.78	Joback Method
dvisc	0.0000022	Pa×s	1200.22	Joback Method
dvisc	0.0000029	Pa×s	1126.00	Joback Method
dvisc	0.0000040	Pa×s	1051.78	Joback Method

dvisc	0.0000057	Pa×s	977.56	Joback Method
dvisc	0.0000086	Pa×s	903.34	Joback Method
dvisc	0.0000141	Pa×s	829.12	Joback Method
dvisc	0.0000254	Pa×s	754.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004205&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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