[1,1'-Biphenyl]-4,4'-dicarboxylic acid, dimethyl ester

Other names: 4,4'-Biphenyldicarboxylic acid, dimethyl ester
Dimethyl 4,4'-biphenyldicarboxylate
Dimethyl biphenyl-4,4'-dicarboxylate
4,4-Dicarboxymethylbiphenyl
4,4'-Bis(methoxycarbonyl)biphenyl
Dimethyl (1,1'-biphenyl)-4,4'-dicarboxylate

Inchi: InChI=1S/C16H14O4/c1-19-15(17)13-7-3-11(4-8-13)12-5-9-14(10-6-12)16(18)20-2/h3-10

InchiKey: BKRIRZXWWALTPU-UHFFFAOYSA-N

Formula: C16H14O4

SMILES: COC(=O)c1ccc(-c2ccc(C(=O)OC)cc2)cc1

Mol. weight [g/mol]: 270.28

CAS: 792-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.44	kJ/mol	Joback Method
hf	-413.05	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	75.40	kJ/mol	Joback Method
ie	9.15 ± 0.05	eV	NIST Webbook
log10ws	-4.56		Crippen Method
logp	2.927		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	781.38	K	Joback Method
tc	1018.00	K	Joback Method
tf	492.28	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.14	J/mol×K	781.38	Joback Method
cpg	612.41	J/mol×K	978.56	Joback Method

cpg	603.68	J/mol×K	939.12	Joback Method
cpg	593.81	J/mol×K	899.69	Joback Method
cpg	582.77	J/mol×K	860.25	Joback Method
cpg	570.55	J/mol×K	820.82	Joback Method
cpg	620.03	J/mol×K	1018.00	Joback Method
dvisc	0.0000953	Pa×s	781.38	Joback Method
dvisc	0.0001178	Pa×s	733.20	Joback Method
dvisc	0.0001500	Pa×s	685.01	Joback Method
dvisc	0.0001981	Pa×s	636.83	Joback Method
dvisc	0.0002738	Pa×s	588.65	Joback Method
dvisc	0.0004009	Pa×s	540.46	Joback Method
dvisc	0.0006325	Pa×s	492.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C792745&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
ie: Ionization energy
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