

Methyl-p-phneylbenzoate

Other names:	4-Biphenylcarboxylic acid, methyl ester Methyl (1,1'-biphenyl)-4-carboxylate Methyl 4-biphenylcarboxylate Methyl p-phenylbenzoate Methyl-4-phenylbenzoate [1,1'-Biphenyl]-4-carboxylic acid, methyl ester p-Phenylbenzoic acid methyl ester
Inchi:	InChI=1S/C14H12O2/c1-16-14(15)13-9-7-12(8-10-13)11-5-3-2-4-6-11/h2-10H,1H3
InchiKey:	GATUGNVDXMYTJX-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	COC(=O)c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	212.25

Physical Properties

Property code	Value	Unit	Source
af	0.5506		Cheméo Relay (1.0)
hf	-167.63	kJ/mol	Cheméo Relay (1.0)
hfus	22.50	kJ/mol	Joback Method
hvap	92.53	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-4.24		Cheméo Relay (1.0)
logp	3.140		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	603.16	K	Cheméo Relay (1.0)
tc	832.46	K	Cheméo Relay (1.0)
tf	390.00 ± 3.00	K	NIST Webbook
vc	0.615	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.01	J/mol×K	654.35	Joback Method
cpg	488.82	J/mol×K	898.02	Joback Method

cpg	479.16	J/mol×K	857.41	Joback Method
cpg	468.50	J/mol×K	816.80	Joback Method
cpg	456.81	J/mol×K	776.19	Joback Method
cpg	444.02	J/mol×K	735.57	Joback Method
cpg	430.11	J/mol×K	694.96	Joback Method
dvisc	0.0003325	Pa×s	519.71	Joback Method
dvisc	0.0001499	Pa×s	654.35	Joback Method
dvisc	0.0001880	Pa×s	609.47	Joback Method
dvisc	0.0002444	Pa×s	564.59	Joback Method
dvisc	0.0012880	Pa×s	385.06	Joback Method
dvisc	0.0004795	Pa×s	474.82	Joback Method
dvisc	0.0007464	Pa×s	429.94	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C720752&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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