3,3'-DIMETHOXYBIPHENYL

Other names: Biphenyl, 3,3'-dimethoxy-
3,3'-Dimethoxybiphenyl
3,3'-dimethoxy-1,1'-biphenyl
Inchi: InChI=1S/C14H14O2/c1-15-13-7-3-5-11(9-13)12-6-4-8-14(10-12)16-2/h3-10H,1-2H3
InchiKey: UCHNVSDXSPIKRG-UHFFFAOYSA-N
Formula: C14H14O2
SMILES: COc1cccc(-c2cccc(OC)c2)c1
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
af	0.5760		Cheméo Relay (1.0)
hf	-97.43	kJ/mol	Cheméo Relay (1.0)
hfus	21.70	kJ/mol	Joback Method
hvap	91.60	kJ/mol	Cheméo Relay (1.0)
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-5.09		Cheméo Relay (1.0)
logp	3.371		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	601.20	K	NIST Webbook
tc	826.65	K	Cheméo Relay (1.0)
tf	338.49	K	Cheméo Relay (1.0)
vc	0.636	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.83	J/mol×K	627.88	Joback Method
cpg	439.04	J/mol×K	666.97	Joback Method
cpg	454.18	J/mol×K	706.05	Joback Method
cpg	468.26	J/mol×K	745.14	Joback Method
cpg	481.31	J/mol×K	784.23	Joback Method
cpg	493.34	J/mol×K	823.31	Joback Method

cpg	504.37	J/mol×K	862.40	Joback Method
dvisc	0.0008710	Pa×s	369.88	Joback Method
dvisc	0.0005193	Pa×s	412.88	Joback Method
dvisc	0.0003413	Pa×s	455.88	Joback Method
dvisc	0.0002411	Pa×s	498.88	Joback Method
dvisc	0.0001800	Pa×s	541.88	Joback Method
dvisc	0.0001403	Pa×s	584.88	Joback Method
dvisc	0.0001132	Pa×s	627.88	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6161508&Units=SI
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):

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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