

4,4'-Dimethoxybiphenyl

Inchi:	InChI=1S/C14H14O2/c1-15-13-7-3-11(4-8-13)12-5-9-14(16-2)10-6-12/h3-10H,1-2H3
InchiKey:	UIMPAOAAAYDUKQ-UHFFFAOYSA-N
Formula:	C14H14O2
SMILES:	COc1ccc(-c2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
hf	-108.86	kJ/mol	Cheméo Relay (1.0)
hfus	21.70	kJ/mol	Joback Method
hvap	90.71	kJ/mol	Cheméo Relay (1.0)
ie	7.66	eV	Cheméo Relay (1.0)
log10ws	-5.01		Cheméo Relay (1.0)
logp	3.371		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	617.45	K	Cheméo Relay (1.0)
tc	826.68	K	Cheméo Relay (1.0)
tf	407.54	K	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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2132801&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):

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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