Diphenyl ether, 4-methoxycarbonyl-3,3'-dimethyl

Inchi: InChI=1S/C16H16O3/c1-11-5-4-6-13(9-11)19-14-7-8-15(12(2)10-14)16(17)18-3/h4-10H,1

InchiKey: RNFNMXQBVGXKKG-UHFFFAOYSA-N

Formula: C16H16O3

SMILES: COC(=O)c1ccc(Oc2cccc(C)c2)cc1C

Mol. weight [g/mol]: 256.30

Physical Properties

Property code	Value	Unit	Source
gf	-59.15	kJ/mol	Joback Method
hf	-311.94	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.882		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	732.49	K	Joback Method
tc	964.63	K	Joback Method
tf	454.87	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.39	J/mol×K	732.49	Joback Method
cpg	557.61	J/mol×K	771.18	Joback Method
cpg	571.68	J/mol×K	809.87	Joback Method
cpg	584.61	J/mol×K	848.56	Joback Method
cpg	596.44	J/mol×K	887.25	Joback Method

cpg	607.15	J/mol×K	925.94	Joback Method
cpg	616.78	J/mol×K	964.63	Joback Method
dvisc	0.0006069	Pa×s	454.87	Joback Method
dvisc	0.0003867	Pa×s	501.14	Joback Method
dvisc	0.0002659	Pa×s	547.41	Joback Method
dvisc	0.0001938	Pa×s	593.68	Joback Method
dvisc	0.0001479	Pa×s	639.95	Joback Method
dvisc	0.0001171	Pa×s	686.22	Joback Method
dvisc	0.0000954	Pa×s	732.49	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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