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

Inchi: InChI=1S/C17H18O3/c1-11-5-6-14(9-12(11)2)20-15-7-8-16(13(3)10-15)17(18)19-4/h5-10

InchiKey: OMPGTWALNLWBCY-UHFFFAOYSA-N

Formula: C17H18O3

SMILES: COC(=O)c1ccc(Oc2ccc(C)c(C)c2)cc1C

Mol. weight [g/mol]: 270.32

Physical Properties

Property code	Value	Unit	Source
gf	-60.36	kJ/mol	Joback Method
hf	-344.05	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.191		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2178.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2178.00		NIST Webbook
tb	760.35	K	Joback Method
tc	989.23	K	Joback Method
tf	478.66	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.46	J/mol×K	760.35	Joback Method
cpg	660.95	J/mol×K	951.09	Joback Method
cpg	650.13	J/mol×K	912.94	Joback Method
cpg	638.18	J/mol×K	874.79	Joback Method
cpg	625.09	J/mol×K	836.64	Joback Method

cpg	610.85	J/mol×K	798.50	Joback Method
cpg	670.65	J/mol×K	989.23	Joback Method
dvisc	0.0000858	Pa×s	760.35	Joback Method
dvisc	0.0001043	Pa×s	713.40	Joback Method
dvisc	0.0001305	Pa×s	666.45	Joback Method
dvisc	0.0001688	Pa×s	619.50	Joback Method
dvisc	0.0002277	Pa×s	572.56	Joback Method
dvisc	0.0003242	Pa×s	525.61	Joback Method
dvisc	0.0004945	Pa×s	478.66	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530408&Units=SI

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