Diphenyl ether, 4,4'-bis-(methoxycarbonyl)-3,3'-dimethyl

Inchi: InChI=1S/C18H18O5/c1-11-9-13(5-7-15(11)17(19)21-3)23-14-6-8-16(12(2)10-14)18(20)2

InchiKey: NOAUOHRDPLEWDZ-UHFFFAOYSA-N

Formula: C18H18O5

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

Mol. weight [g/mol]: 314.33

Physical Properties

Property code	Value	Unit	Source
gf	-285.86	kJ/mol	Joback Method
hf	-609.49	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	83.58	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.669		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2434.00		NIST Webbook
rinpol	2413.00		NIST Webbook
rinpol	2427.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	859.52	K	Joback Method
tc	1088.44	K	Joback Method
tf	562.09	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.94	J/mol×K	859.52	Joback Method
cpg	742.67	J/mol×K	1050.29	Joback Method
cpg	735.01	J/mol×K	1012.13	Joback Method
cpg	726.00	J/mol×K	973.98	Joback Method
cpg	715.64	J/mol×K	935.83	Joback Method

cpg	703.96	J/mol×K	897.67	Joback Method
cpg	748.97	J/mol×K	1088.44	Joback Method
dvisc	0.0000580	Pa×s	859.52	Joback Method
dvisc	0.0000705	Pa×s	809.95	Joback Method
dvisc	0.0000878	Pa×s	760.38	Joback Method
dvisc	0.0001127	Pa×s	710.81	Joback Method
dvisc	0.0001502	Pa×s	661.23	Joback Method
dvisc	0.0002098	Pa×s	611.66	Joback Method
dvisc	0.0003109	Pa×s	562.09	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=R530379&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