Diphenyl ether, 3,4,4'-tris-(methoxycarbonyl)-3'-methyl

Inchi: InChI=1S/C19H18O7/c1-11-9-12(5-7-14(11)17(20)23-2)26-13-6-8-15(18(21)24-3)16(10-1

InchiKey: WOAHMADQCWPWEN-UHFFFAOYSA-N

Formula: C19H18O7

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

Mol. weight [g/mol]: 358.34

Physical Properties

Property code	Value	Unit	Source
gf	-511.36	kJ/mol	Joback Method
hf	-874.93	kJ/mol	Joback Method
hfus	41.04	kJ/mol	Joback Method
hvap	94.97	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.147		Crippen Method
mcvol	259.240	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2609.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	958.69	K	Joback Method
tc	1191.32	K	Joback Method
tf	645.52	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.04	J/mol×K	958.69	Joback Method
cpg	813.29	J/mol×K	1152.55	Joback Method
cpg	810.22	J/mol×K	1113.78	Joback Method
cpg	805.43	J/mol×K	1075.01	Joback Method
cpg	798.96	J/mol×K	1036.23	Joback Method
cpg	790.82	J/mol×K	997.46	Joback Method

cpg	814.61	J/mol×K	1191.32	Joback Method
dvisc	0.0000370	Pa×s	958.69	Joback Method
dvisc	0.0000448	Pa×s	906.50	Joback Method
dvisc	0.0000555	Pa×s	854.30	Joback Method
dvisc	0.0000708	Pa×s	802.11	Joback Method
dvisc	0.0000934	Pa×s	749.91	Joback Method
dvisc	0.0001283	Pa×s	697.72	Joback Method
dvisc	0.0001857	Pa×s	645.52	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R530344&Units=SI
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

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

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