4-Methoxybenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C20H16O3/c1-22-18-11-9-17(10-12-18)20(21)23-19-13-7-16(8-14-19)15-5-3-2
InchiKey: QXSYNKWEBROFDJ-UHFFFAOYSA-N
Formula: C20H16O3
SMILES: COc1ccc(C(=O)Oc2ccc(-c3ccccc3)cc2)cc1
Mol. weight [g/mol]: 304.34

Physical Properties

Property code	Value	Unit	Source
gf	96.57	kJ/mol	Joback Method
hf	-146.50	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.581		Crippen Method
mcvol	234.690	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	2867.00		NIST Webbook
tb	845.71	K	Joback Method
tc	1099.79	K	Joback Method
tf	513.85	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.17	J/mol×K	845.71	Joback Method
cpg	727.63	J/mol×K	1057.44	Joback Method
cpg	718.93	J/mol×K	1015.09	Joback Method
cpg	708.90	J/mol×K	972.75	Joback Method
cpg	697.47	J/mol×K	930.40	Joback Method
cpg	684.58	J/mol×K	888.06	Joback Method
cpg	735.05	J/mol×K	1099.79	Joback Method
dvisc	0.0000601	Pa×s	845.71	Joback Method
dvisc	0.0000750	Pa×s	790.40	Joback Method

dvisc	0.0000968	Pa×s	735.09	Joback Method
dvisc	0.0001303	Pa×s	679.78	Joback Method
dvisc	0.0001848	Pa×s	624.47	Joback Method
dvisc	0.0002805	Pa×s	569.16	Joback Method
dvisc	0.0004657	Pa×s	513.85	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=U360533&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