2-Chlorobenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C19H13ClO2/c20-18-9-5-4-8-17(18)19(21)22-16-12-10-15(11-13-16)14-6-2-1-3
InchiKey: PICQCEDMAHLCPV-UHFFFAOYSA-N
Formula: C19H13ClO2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1ccccc1Cl
Mol. weight [g/mol]: 308.76

Physical Properties

Property code	Value	Unit	Source
gf	181.22	kJ/mol	Joback Method
hf	-9.38	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.226		Crippen Method
mcvol	226.970	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	2735.00		NIST Webbook
tb	837.84	K	Joback Method
tc	1102.95	K	Joback Method
tf	510.27	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.13	J/mol×K	837.84	Joback Method
cpg	624.56	J/mol×K	882.02	Joback Method
cpg	636.56	J/mol×K	926.21	Joback Method
cpg	647.24	J/mol×K	970.39	Joback Method
cpg	656.67	J/mol×K	1014.58	Joback Method
cpg	664.97	J/mol×K	1058.76	Joback Method
cpg	672.23	J/mol×K	1102.95	Joback Method
dvisc	0.0006004	Pa×s	510.27	Joback Method
dvisc	0.0003644	Pa×s	564.87	Joback Method

dvisc	0.0002415	Pa×s	619.46	Joback Method
dvisc	0.0001711	Pa×s	674.06	Joback Method
dvisc	0.0001276	Pa×s	728.65	Joback Method
dvisc	0.0000991	Pa×s	783.25	Joback Method
dvisc	0.0000796	Pa×s	837.84	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=U360530&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