3-Chlorobenzoic acid, phenyl ester

Inchi: InChI=1S/C13H9ClO2/c14-11-6-4-5-10(9-11)13(15)16-12-7-2-1-3-8-12/h1-9H
InchiKey: BVSINJUGJASNKK-UHFFFAOYSA-N
Formula: C13H9ClO2
SMILES: O=C(Oc1ccccc1)c1cccc(Cl)c1
Mol. weight [g/mol]: 232.66

Physical Properties

Property code	Value	Unit	Source
gf	27.92	kJ/mol	Joback Method
hf	-110.60	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	63.29	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.559		Crippen Method
mcvol	166.190	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1876.00		NIST Webbook
tb	668.90	K	Joback Method
tc	920.71	K	Joback Method
tf	403.71	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.69	J/mol×K	668.90	Joback Method
cpg	402.92	J/mol×K	710.87	Joback Method
cpg	415.01	J/mol×K	752.84	Joback Method
cpg	426.00	J/mol×K	794.80	Joback Method
cpg	435.96	J/mol×K	836.77	Joback Method
cpg	444.92	J/mol×K	878.74	Joback Method
cpg	452.94	J/mol×K	920.71	Joback Method
dvisc	0.0012209	Pa×s	403.71	Joback Method
dvisc	0.0007326	Pa×s	447.91	Joback Method

dvisc	0.0004818	Pa×s	492.11	Joback Method
dvisc	0.0003395	Pa×s	536.31	Joback Method
dvisc	0.0002524	Pa×s	580.50	Joback Method
dvisc	0.0001956	Pa×s	624.70	Joback Method
dvisc	0.0001568	Pa×s	668.90	Joback Method

Sources

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=U357783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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