3-Chlorobenzoic acid, cyclohexyl ester

Inchi: InChI=1S/C13H15ClO2/c14-11-6-4-5-10(9-11)13(15)16-12-7-2-1-3-8-12/h4-6,9,12H,1-3,7
InchiKey: ZTIHECJKSNZAQC-UHFFFAOYSA-N
Formula: C13H15ClO2
SMILES: O=C(OC1CCCCC1)c1cccc(Cl)c1
Mol. weight [g/mol]: 238.71

Physical Properties

Property code	Value	Unit	Source
gf	-60.04	kJ/mol	Joback Method
hf	-292.81	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.830		Crippen Method
mcvol	179.090	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1836.00		NIST Webbook
tb	661.77	K	Joback Method
tc	905.78	K	Joback Method
tf	384.67	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.22	J/mol×K	661.77	Joback Method
cpg	479.76	J/mol×K	702.44	Joback Method
cpg	495.95	J/mol×K	743.11	Joback Method
cpg	510.81	J/mol×K	783.78	Joback Method
cpg	524.39	J/mol×K	824.45	Joback Method
cpg	536.74	J/mol×K	865.11	Joback Method
cpg	547.88	J/mol×K	905.78	Joback Method
dvisc	0.0017801	Pa×s	384.67	Joback Method
dvisc	0.0009695	Pa×s	430.85	Joback Method

dvisc	0.0005940	Pa×s	477.04	Joback Method
dvisc	0.0003968	Pa×s	523.22	Joback Method
dvisc	0.0002830	Pa×s	569.40	Joback Method
dvisc	0.0002123	Pa×s	615.59	Joback Method
dvisc	0.0001658	Pa×s	661.77	Joback Method

Sources

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=U357782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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