2-Chlorobenzoic acid, benzyl ester

Other names: Benzyl 2-chlorobenzoate
Inchi: InChI=1S/C14H11ClO2/c15-13-9-5-4-8-12(13)14(16)17-10-11-6-2-1-3-7-11/h1-9H,10H2
InchiKey: IJIVXOPMPSQRSF-UHFFFAOYSA-N
Formula: C14H11ClO2
SMILES: O=C(OCc1ccccc1)c1ccccc1Cl
Mol. weight [g/mol]: 246.69
CAS: 7579-40-0

Physical Properties

Property code	Value	Unit	Source
gf	36.34	kJ/mol	Joback Method
hf	-131.24	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	65.51	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.697		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1904.00		NIST Webbook
rinpol	1867.00		NIST Webbook
ripol	2833.00		NIST Webbook
ripol	2869.00		NIST Webbook
ripol	2905.00		NIST Webbook
ripol	2877.00		NIST Webbook
ripol	2865.00		NIST Webbook
ripol	2833.00		NIST Webbook
tb	691.78	K	Joback Method
tc	938.00	K	Joback Method
tf	414.98	K	Joback Method

vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.76	J/mol×K	691.78	Joback Method
cpg	453.56	J/mol×K	732.82	Joback Method
cpg	466.19	J/mol×K	773.85	Joback Method
cpg	477.72	J/mol×K	814.89	Joback Method
cpg	488.18	J/mol×K	855.92	Joback Method
cpg	497.64	J/mol×K	896.96	Joback Method
cpg	506.14	J/mol×K	938.00	Joback Method
dvisc	0.0011566	Pa×s	414.98	Joback Method
dvisc	0.0006831	Pa×s	461.11	Joback Method
dvisc	0.0004441	Pa×s	507.25	Joback Method
dvisc	0.0003102	Pa×s	553.38	Joback Method
dvisc	0.0002289	Pa×s	599.51	Joback Method
dvisc	0.0001765	Pa×s	645.65	Joback Method
dvisc	0.0001408	Pa×s	691.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7579400&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume