Benzyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, phenylmethyl ester
Inchi: InChI=1S/C14H11ClO2/c15-13-8-4-7-12(9-13)14(16)17-10-11-5-2-1-3-6-11/h1-9H,10H2
InchiKey: FKQRAQQDDUKITH-UHFFFAOYSA-N
Formula: C14H11ClO2
SMILES: O=C(OCc1ccccc1)c1cccc(Cl)c1
Mol. weight [g/mol]: 246.69

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	1897.00		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1942.00		NIST Webbook
ripol	2768.00		NIST Webbook
ripol	2786.00		NIST Webbook
ripol	2799.00		NIST Webbook
ripol	2768.00		NIST Webbook
ripol	2799.00		NIST Webbook
ripol	2831.00		NIST Webbook
ripol	2797.00		NIST Webbook
ripol	2737.00		NIST Webbook
ripol	2768.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373600&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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