Benzyl chloroformate

Other names:	Cbz chloride
	Carbobenzoxy chloride
	Carbonochloridic acid, phenylmethyl ester
	Benzyl carbonochloridate
	Benzyl chlorocarbonate
	Benzyloxycarbonyl chloride
	Carbobenzyloxy chloride
	Chloroformic acid, benzyl ester
	Formic acid, chloro-, benzyl ester
	BZCF
	UN 1739
	Benzylcarbonyl chloride
	Chloroformic acid, phenylmethyl ester
	NSC 83466
Inchi:	InChI=1S/C8H7ClO2/c9-8(10)11-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	HSDAJNMJOMSNEV-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	O=C(Cl)OCc1ccccc1
Mol. weight [g/mol]:	170.59
CAS:	501-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-116.96	kJ/mol	Joback Method
hf	-232.46	kJ/mol	Joback Method
hfl	-376.20 ± 1.10	kJ/mol	NIST Webbook
hfus	17.50	kJ/mol	Joback Method
hvap	38.50 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.76		Crippen Method
logp	2.562		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	522.84	K	Joback Method
tc	747.81	K	Joback Method
tf	308.42	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.13	J/mol×K	522.84	Joback Method
cpg	248.91	J/mol×K	560.34	Joback Method
cpg	259.02	J/mol×K	597.83	Joback Method
cpg	268.46	J/mol×K	635.33	Joback Method
cpg	277.26	J/mol×K	672.82	Joback Method
cpg	285.43	J/mol×K	710.32	Joback Method
cpg	292.99	J/mol×K	747.81	Joback Method
dvisc	0.0022365	Pa×s	308.42	Joback Method
dvisc	0.0012890	Pa×s	344.16	Joback Method
dvisc	0.0008240	Pa×s	379.89	Joback Method
dvisc	0.0005689	Pa×s	415.63	Joback Method
dvisc	0.0004165	Pa×s	451.37	Joback Method
dvisc	0.0003192	Pa×s	487.10	Joback Method
dvisc	0.0002537	Pa×s	522.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C501531&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
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume