2-Iodobenzyl chloride

Other names:	Benzene, 1-(chloromethyl)-2-iodo-
	1-(chloromethyl)-2-iodobenzene
Inchi:	InChI=1S/C7H6ClI/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2
InchiKey:	FTMNWZHKQGKKAU-UHFFFAOYSA-N
Formula:	C7H6ClI
SMILES:	ClCc1ccccc1I
Mol. weight [g/mol]:	252.48
CAS:	59473-45-9

Physical Properties

Property code	Value	Unit	Source
gf	157.03	kJ/mol	Joback Method
hf	98.38	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	47.87	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.030		Crippen Method
mcvol	123.790	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	521.79	K	Joback Method
tc	780.35	K	Joback Method
tf	295.57	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.27	J/mol×K	521.79	Joback Method
cpg	213.94	J/mol×K	564.88	Joback Method
cpg	222.80	J/mol×K	607.98	Joback Method
cpg	230.92	J/mol×K	651.07	Joback Method
cpg	238.34	J/mol×K	694.17	Joback Method
cpg	245.14	J/mol×K	737.26	Joback Method
cpg	251.36	J/mol×K	780.35	Joback Method

dvisc	0.0027681	Pa×s	295.57	Joback Method
dvisc	0.0015719	Pa×s	333.27	Joback Method
dvisc	0.0010014	Pa×s	370.98	Joback Method
dvisc	0.0006933	Pa×s	408.68	Joback Method
dvisc	0.0005108	Pa×s	446.38	Joback Method
dvisc	0.0003946	Pa×s	484.09	Joback Method
dvisc	0.0003165	Pa×s	521.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	4.30	NIST Webbook

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=C59473459&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume