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

Physical Properties

Property code	Value	Unit	Source
hf	112.74	kJ/mol	Cheméo Relay (1.0)
hfus	16.14	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-3.84		Cheméo Relay (1.0)
logp	3.030		Crippen Method
mcvol	123.790	ml/mol	McGowan Method
tb	531.11	K	Cheméo Relay (1.0)
tf	287.91	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59473459&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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