3-Chloro-2-iodotoluene

Other names: 3-Chloro-2-iodotoluene
Inchi: InChI=1S/C7H6ClI/c1-5-3-2-4-6(8)7(5)9/h2-4H,1H3
InchiKey: FTGLKPMFTLNUBN-UHFFFAOYSA-N
Formula: C7H6ClI
SMILES: Cc1cccc(Cl)c1I
Mol. weight [g/mol]: 252.48

Physical Properties

Property code	Value	Unit	Source
af	0.3124		Cheméo Relay (1.0)
gf	147.40	kJ/mol	Joback Method
hf	116.20	kJ/mol	Cheméo Relay (1.0)
hfus	15.75	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-4.23		Cheméo Relay (1.0)
logp	3.253		Crippen Method
mcvol	123.790	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	519.76	K	Cheméo Relay (1.0)
tc	768.19	K	Cheméo Relay (1.0)
tf	287.58	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.36	J/mol×K	526.77	Joback Method
cpg	249.10	J/mol×K	786.63	Joback Method
cpg	242.95	J/mol×K	743.32	Joback Method
cpg	236.27	J/mol×K	700.01	Joback Method
cpg	229.02	J/mol×K	656.70	Joback Method
cpg	221.15	J/mol×K	613.39	Joback Method
cpg	212.62	J/mol×K	570.08	Joback Method

dvisc	0.0006244	Pa×s	417.43	Joback Method
dvisc	0.0003071	Pa×s	526.77	Joback Method
dvisc	0.0003756	Pa×s	490.32	Joback Method
dvisc	0.0004745	Pa×s	453.88	Joback Method
dvisc	0.0021012	Pa×s	308.09	Joback Method
dvisc	0.0008661	Pa×s	380.98	Joback Method
dvisc	0.0012872	Pa×s	344.54	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5100981&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume