4-Chloro-2-iodotoluene

Inchi: InChI=1S/C7H6ClI/c1-5-2-3-6(8)4-7(5)9/h2-4H,1H3
InchiKey: ZIOGCIPQDRCAKY-UHFFFAOYSA-N
Formula: C7H6ClI
SMILES: Cc1ccc(Cl)cc1I
Mol. weight [g/mol]: 252.48

Physical Properties

Property code	Value	Unit	Source
hf	116.04	kJ/mol	Cheméo Relay (1.0)
hfus	15.75	kJ/mol	Joback Method
hvap	58.64	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
logp	3.253		Crippen Method
mcvol	123.790	ml/mol	McGowan Method
tb	515.70	K	NIST Webbook
tf	294.95	K	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	212.62	J/mol×K	570.08	Joback Method
cpg	221.15	J/mol×K	613.39	Joback Method
cpg	229.02	J/mol×K	656.70	Joback Method
cpg	236.27	J/mol×K	700.01	Joback Method
cpg	242.95	J/mol×K	743.32	Joback Method
cpg	249.10	J/mol×K	786.63	Joback Method
dvisc	0.0021012	Pa×s	308.09	Joback Method
dvisc	0.0012872	Pa×s	344.54	Joback Method
dvisc	0.0008661	Pa×s	380.98	Joback Method
dvisc	0.0006244	Pa×s	417.43	Joback Method
dvisc	0.0004745	Pa×s	453.88	Joback Method
dvisc	0.0003756	Pa×s	490.32	Joback Method
dvisc	0.0003071	Pa×s	526.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	0.90	NIST Webbook

Sources

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=C33184484&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

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
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