1-Chloro-2-iodoethane

Other names: 1,2-Chloroiodoethane
1-Chloro-2-iodoethane
Inchi: InChI=1S/C2H4ClI/c3-1-2-4/h1-2H2
InchiKey: JTWWWQGSFTWWDL-UHFFFAOYSA-N
Formula: C2H4ClI
SMILES: ClCCI
Mol. weight [g/mol]: 190.41

Physical Properties

Property code	Value	Unit	Source
af	0.2392		Cheméo Relay (1.0)
gf	12.15	kJ/mol	Joback Method
hf	-47.70 ± 5.00	kJ/mol	NIST Webbook
hfus	9.54	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.660		Crippen Method
mcvol	77.100	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	411.66	K	Cheméo Relay (1.0)
tc	670.36	K	Cheméo Relay (1.0)
tf	279.81	K	Cheméo Relay (1.0)
vc	0.272	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.57	J/mol×K	375.73	Joback Method
cpg	114.83	J/mol×K	592.51	Joback Method
cpg	111.73	J/mol×K	556.38	Joback Method
cpg	108.40	J/mol×K	520.25	Joback Method
cpg	104.84	J/mol×K	484.12	Joback Method
cpg	101.03	J/mol×K	447.99	Joback Method

cpg	96.94	J/mol×K	411.86	Joback Method
dvisc	0.0010829	Pa×s	288.00	Joback Method
dvisc	0.0004716	Pa×s	375.73	Joback Method
dvisc	0.0005937	Pa×s	346.49	Joback Method
dvisc	0.0007799	Pa×s	317.25	Joback Method
dvisc	0.0051514	Pa×s	200.28	Joback Method
dvisc	0.0016193	Pa×s	258.76	Joback Method
dvisc	0.0026830	Pa×s	229.52	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=C624704&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