Hexamethylenechloroiodide

Other names: 1-Chloro-6-iodohexane
Hexane, 1-chloro-6-iodo-
Inchi: InChI=1S/C6H12ClI/c7-5-3-1-2-4-6-8/h1-6H2
InchiKey: QTJHNJCILMMRIQ-UHFFFAOYSA-N
Formula: C6H12ClI
SMILES: ClCCCCCCI
Mol. weight [g/mol]: 246.52

Physical Properties

Property code	Value	Unit	Source
af	0.4314		Cheméo Relay (1.0)
hf	-108.25	kJ/mol	Cheméo Relay (1.0)
hfus	19.90	kJ/mol	Joback Method
hvap	61.27	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-4.17		Cheméo Relay (1.0)
logp	3.221		Crippen Method
mcvol	133.460	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	493.80	K	Cheméo Relay (1.0)
tc	719.52	K	Cheméo Relay (1.0)
tf	249.05	K	Cheméo Relay (1.0)
vc	0.483	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.36	J/mol×K	467.25	Joback Method
cpg	289.37	J/mol×K	674.20	Joback Method
cpg	281.45	J/mol×K	639.71	Joback Method
cpg	273.07	J/mol×K	605.22	Joback Method
cpg	264.20	J/mol×K	570.73	Joback Method
cpg	254.80	J/mol×K	536.23	Joback Method
cpg	244.87	J/mol×K	501.74	Joback Method

dvisc	0.0009198	Pa×s	356.31	Joback Method
dvisc	0.0003613	Pa×s	467.25	Joback Method
dvisc	0.0004676	Pa×s	430.27	Joback Method
dvisc	0.0006353	Pa×s	393.29	Joback Method
dvisc	0.0054511	Pa×s	245.36	Joback Method
dvisc	0.0014509	Pa×s	319.32	Joback Method
dvisc	0.0025788	Pa×s	282.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34683733&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume