Cyclohexene, 1-iodo-2-methyl-

Inchi: InChI=1S/C7H11I/c1-6-4-2-3-5-7(6)8/h2-5H2,1H3
InchiKey: YPYNZJFLYQQPLF-UHFFFAOYSA-N
Formula: C7H11I
SMILES: CC1=C(I)CCCC1
Mol. weight [g/mol]: 222.07
CAS: 40648-08-6

Physical Properties

Property code	Value	Unit	Source
gf	109.04	kJ/mol	Joback Method
hf	-1.44	kJ/mol	Joback Method
hfus	9.50	kJ/mol	Joback Method
hvap	42.90	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.269		Crippen Method
mcvol	120.150	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1185.00		NIST Webbook
tb	486.04	K	Joback Method
tc	733.80	K	Joback Method
tf	264.13	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.10	J/mol×K	486.04	Joback Method
cpg	228.65	J/mol×K	527.33	Joback Method
cpg	241.29	J/mol×K	568.63	Joback Method
cpg	253.09	J/mol×K	609.92	Joback Method
cpg	264.07	J/mol×K	651.22	Joback Method
cpg	274.29	J/mol×K	692.51	Joback Method
cpg	283.79	J/mol×K	733.80	Joback Method
dvisc	0.0043566	Pa×s	264.13	Joback Method

dvisc	0.0021701	Pa×s	301.12	Joback Method
dvisc	0.0012590	Pa×s	338.10	Joback Method
dvisc	0.0008132	Pa×s	375.08	Joback Method
dvisc	0.0005682	Pa×s	412.07	Joback Method
dvisc	0.0004211	Pa×s	449.05	Joback Method
dvisc	0.0003267	Pa×s	486.04	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40648086&Units=SI
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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume