Cyclohexene, 4-iodo-3-methyl

Inchi: InChI=1S/C7H11I/c1-6-4-2-3-5-7(6)8/h2,4,6-7H,3,5H2,1H3
InchiKey: QIRACRDZOORENZ-UHFFFAOYSA-N
Formula: C7H11I
SMILES: CC1C=CCCC1I
Mol. weight [g/mol]: 222.07

Physical Properties

Property code	Value	Unit	Source
gf	112.88	kJ/mol	Joback Method
hf	-19.18	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	40.96	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.776		Crippen Method
mcvol	120.150	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1153.00		NIST Webbook
tb	466.74	K	Joback Method
tc	711.31	K	Joback Method
tf	230.61	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.79	J/mol×K	466.74	Joback Method
cpg	284.03	J/mol×K	670.55	Joback Method
cpg	272.43	J/mol×K	629.79	Joback Method
cpg	259.95	J/mol×K	589.03	Joback Method
cpg	246.55	J/mol×K	548.26	Joback Method
cpg	232.17	J/mol×K	507.50	Joback Method
cpg	294.77	J/mol×K	711.31	Joback Method
dvisc	0.0003817	Pa×s	466.74	Joback Method
dvisc	0.0004748	Pa×s	427.38	Joback Method

dvisc	0.0006173	Pa×s	388.03	Joback Method
dvisc	0.0008514	Pa×s	348.68	Joback Method
dvisc	0.0012747	Pa×s	309.32	Joback Method
dvisc	0.0021465	Pa×s	269.97	Joback Method
dvisc	0.0043183	Pa×s	230.61	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R25487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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