

Cyclohexene, 3-iodo-4-methyl

Inchi:	InChI=1S/C7H11I/c1-6-4-2-3-5-7(6)8/h3,5-7H,2,4H2,1H3
InchiKey:	HGSYKHQOZSFUOW-UHFFFAOYSA-N
Formula:	C7H11I
SMILES:	CC1CCC=CC1I
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
mvol	120.150	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1152.00		NIST Webbook
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tb	466.74	K	Joback Method
tc	711.31	K	Joback Method
tf	230.61	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.79	J/mol×K	466.74	Joback Method
cpg	232.17	J/mol×K	507.50	Joback Method
cpg	246.55	J/mol×K	548.26	Joback Method
cpg	259.95	J/mol×K	589.03	Joback Method
cpg	272.43	J/mol×K	629.79	Joback Method
cpg	284.03	J/mol×K	670.55	Joback Method
cpg	294.77	J/mol×K	711.31	Joback Method
dvisc	0.0043183	Paxs	230.61	Joback Method

dvisc	0.0021465	Paxs	269.97	Joback Method
dvisc	0.0012747	Paxs	309.32	Joback Method
dvisc	0.0008514	Paxs	348.68	Joback Method
dvisc	0.0006173	Paxs	388.03	Joback Method
dvisc	0.0004748	Paxs	427.38	Joback Method
dvisc	0.0003817	Paxs	466.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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