

Cyclohexane, 1-iodo-2-methyl

Inchi:	InChI=1S/C7H13I/c1-6-4-2-3-5-7(6)8/h6-7H,2-5H2,1H3
InchiKey:	YAGDYJMIKDUXJQ-UHFFFAOYSA-N
Formula:	C7H13I
SMILES:	CC1CCCCC1I
Mol. weight [g/mol]:	224.08

Physical Properties

Property code	Value	Unit	Source
gf	82.92	kJ/mol	Joback Method
hf	-76.96	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	40.67	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.000		Crippen Method
mcvol	124.450	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinsol	1135.00		NIST Webbook
tb	467.58	K	Joback Method
tc	709.49	K	Joback Method
tf	229.85	K	Joback Method
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.32	J/molxK	467.58	Joback Method
cpg	249.15	J/molxK	507.90	Joback Method
cpg	264.94	J/molxK	548.22	Joback Method
cpg	279.71	J/molxK	588.53	Joback Method
cpg	293.52	J/molxK	628.85	Joback Method
cpg	306.39	J/molxK	669.17	Joback Method
cpg	318.36	J/molxK	709.49	Joback Method
dvisc	0.0055420	Paxs	229.85	Joback Method
dvisc	0.0025695	Paxs	269.47	Joback Method

dvisc	0.0014509	Paxs	309.09	Joback Method
dvisc	0.0009328	Paxs	348.71	Joback Method
dvisc	0.0006563	Paxs	388.34	Joback Method
dvisc	0.0004928	Paxs	427.96	Joback Method
dvisc	0.0003885	Paxs	467.58	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=R25423&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

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