

1,3-Cyclohexadiene, 1-iodo

Inchi:	InChI=1S/C6H7I/c7-6-4-2-1-3-5-6/h1-2,4H,3,5H2
InchiKey:	ZWRMMMHEMAELAF-UHFFFAOYSA-N
Formula:	C6H7I
SMILES:	IC1=CC=CCC1
Mol. weight [g/mol]:	206.02

Physical Properties

Property code	Value	Unit	Source
gf	140.21	kJ/mol	Joback Method
hf	88.45	kJ/mol	Joback Method
hfus	8.52	kJ/mol	Joback Method
hvap	40.31	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.655		Crippen Method
mcvol	101.760	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
rinpol	1077.00		NIST Webbook
tb	457.34	K	Joback Method
tc	711.17	K	Joback Method
tf	241.10	K	Joback Method
vc	0.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.33	J/molxK	457.34	Joback Method
cpg	170.50	J/molxK	499.64	Joback Method
cpg	180.78	J/molxK	541.95	Joback Method
cpg	190.23	J/molxK	584.25	Joback Method
cpg	198.92	J/molxK	626.56	Joback Method
cpg	206.89	J/molxK	668.86	Joback Method
cpg	214.20	J/molxK	711.17	Joback Method
dvisc	0.0052623	Paxs	241.10	Joback Method
dvisc	0.0025270	Paxs	277.14	Joback Method

dvisc	0.0014366	Paxs	313.18	Joback Method
dvisc	0.0009177	Paxs	349.22	Joback Method
dvisc	0.0006375	Paxs	385.26	Joback Method
dvisc	0.0004714	Paxs	421.30	Joback Method
dvisc	0.0003655	Paxs	457.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R25231&Units=SI

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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