

1,4-Cyclohexadiene, 6-iodo

Inchi:	InChI=1S/C6H7I/c7-6-4-2-1-3-5-6/h2-6H,1H2
InchiKey:	QFWMAPLHMRXMCV-UHFFFAOYSA-N
Formula:	C6H7I
SMILES:	IC1C=CCC=C1
Mol. weight [g/mol]:	206.02

Physical Properties

Property code	Value	Unit	Source
gf	142.13	kJ/mol	Joback Method
hf	79.58	kJ/mol	Joback Method
hfus	9.98	kJ/mol	Joback Method
hvap	39.34	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.306		Crippen Method
mcvol	101.760	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
rinsol	1121.00		NIST Webbook
tb	447.69	K	Joback Method
tc	699.71	K	Joback Method
tf	224.34	K	Joback Method
vc	0.364	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.44	J/molxK	447.69	Joback Method
cpg	172.57	J/molxK	489.69	Joback Method
cpg	183.76	J/molxK	531.70	Joback Method
cpg	194.07	J/molxK	573.70	Joback Method
cpg	203.53	J/molxK	615.71	Joback Method
cpg	212.22	J/molxK	657.71	Joback Method
cpg	220.18	J/molxK	699.71	Joback Method
dvisc	0.0051624	Paxs	224.34	Joback Method
dvisc	0.0024676	Paxs	261.56	Joback Method

dvisc	0.0014177	Paxs	298.79	Joback Method
dvisc	0.0009209	Paxs	336.01	Joback Method
dvisc	0.0006520	Paxs	373.24	Joback Method
dvisc	0.0004914	Paxs	410.47	Joback Method
dvisc	0.0003882	Paxs	447.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25398&Units=SI
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

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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