

1,4-Cyclohexadiene, 2-iodo-1-methyl

Inchi:	InChI=1S/C7H9I/c1-6-4-2-3-5-7(6)8/h2-3H,4-5H2,1H3
InchiKey:	AWKLVHINESMFFT-UHFFFAOYSA-N
Formula:	C7H9I
SMILES:	CC1=C(I)CC=CC1
Mol. weight [g/mol]:	220.05

Physical Properties

Property code	Value	Unit	Source
gf	139.00	kJ/mol	Joback Method
hf	56.34	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	43.20	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.045		Crippen Method
mcvol	115.850	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1231.00		NIST Webbook
tb	485.20	K	Joback Method
tc	735.69	K	Joback Method
tf	264.89	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.90	J/molxK	485.20	Joback Method
cpg	251.08	J/molxK	693.94	Joback Method
cpg	242.15	J/molxK	652.19	Joback Method
cpg	232.52	J/molxK	610.45	Joback Method
cpg	222.13	J/molxK	568.70	Joback Method
cpg	210.94	J/molxK	526.95	Joback Method
cpg	259.34	J/molxK	735.69	Joback Method
dvisc	0.0003237	Paxs	485.20	Joback Method

dvisc	0.0004101	Paxs	448.48	Joback Method
dvisc	0.0005421	Paxs	411.76	Joback Method
dvisc	0.0007567	Paxs	375.04	Joback Method
dvisc	0.0011357	Paxs	338.33	Joback Method
dvisc	0.0018814	Paxs	301.61	Joback Method
dvisc	0.0035851	Paxs	264.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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