

1,3-Cyclohexadiene, 5-iodo-6-methyl

Inchi:	InChI=1S/C7H9I/c1-6-4-2-3-5-7(6)8/h2-7H,1H3
InchiKey:	SOWPUUFIAMNFLX-UHFFFAOYSA-N
Formula:	C7H9I
SMILES:	CC1C=CC=CC1I
Mol. weight [g/mol]:	220.05

Physical Properties

Property code	Value	Unit	Source
gf	142.84	kJ/mol	Joback Method
hf	38.60	kJ/mol	Joback Method
hfus	13.64	kJ/mol	Joback Method
hvap	41.25	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.552		Crippen Method
mcvol	115.850	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinsol	1151.00		NIST Webbook
tb	465.90	K	Joback Method
tc	713.18	K	Joback Method
tf	231.37	K	Joback Method
vc	0.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.34	J/molxK	465.90	Joback Method
cpg	215.23	J/molxK	507.11	Joback Method
cpg	228.16	J/molxK	548.33	Joback Method
cpg	240.16	J/molxK	589.54	Joback Method
cpg	251.29	J/molxK	630.76	Joback Method
cpg	261.58	J/molxK	671.97	Joback Method
cpg	271.08	J/molxK	713.18	Joback Method
dvisc	0.0033740	Paxs	231.37	Joback Method
dvisc	0.0017953	Paxs	270.46	Joback Method

dvisc	0.0011203	Paxs	309.55	Joback Method
dvisc	0.0007771	Paxs	348.63	Joback Method
dvisc	0.0005802	Paxs	387.72	Joback Method
dvisc	0.0004571	Paxs	426.81	Joback Method
dvisc	0.0003748	Paxs	465.90	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=R25295&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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