

1,4-Cyclohexadiene, 1-iodo-6-methyl

Inchi:	InChI=1S/C7H9I/c1-6-4-2-3-5-7(6)8/h2,4-6H,3H2,1H3
InchiKey:	YFMZAAFLWVXEI-UHFFFAOYSA-N
Formula:	C7H9I
SMILES:	CC1C=CCC=C1I
Mol. weight [g/mol]:	220.05

Physical Properties

Property code	Value	Unit	Source
gf	140.92	kJ/mol	Joback Method
hf	47.47	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	42.22	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.901		Crippen Method
mcvol	115.850	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinsol	1203.00		NIST Webbook
tb	475.55	K	Joback Method
tc	724.48	K	Joback Method
tf	248.13	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.34	J/mol×K	475.55	Joback Method
cpg	256.50	J/mol×K	682.99	Joback Method
cpg	246.90	J/mol×K	641.50	Joback Method
cpg	236.54	J/mol×K	600.01	Joback Method
cpg	225.35	J/mol×K	558.53	Joback Method
cpg	213.30	J/mol×K	517.04	Joback Method
cpg	265.37	J/mol×K	724.48	Joback Method
dvisc	0.0003509	Paxs	475.55	Joback Method
dvisc	0.0004371	Paxs	437.65	Joback Method

dvisc	0.0005676	Paxs	399.74	Joback Method
dvisc	0.0007787	Paxs	361.84	Joback Method
dvisc	0.0011503	Paxs	323.94	Joback Method
dvisc	0.0018843	Paxs	286.03	Joback Method
dvisc	0.0035890	Paxs	248.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25366&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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