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

Inchi: InChI=1S/C7H9I/c1-6-4-2-3-5-7(6)8/h2-4,7H,5H2,1H3
InchiKey: YTOJCIZZFOUWST-UHFFFAOYSA-N
Formula: C7H9I
SMILES: CC1=CC=CCC1I
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	-3.41		Crippen Method
logp	2.696		Crippen Method
mcvol	115.850	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	1179.00		NIST Webbook
tb	475.55	K	Joback Method
tc	724.48	K	Joback Method
tf	248.13	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.34	J/mol×K	475.55	Joback Method
cpg	213.30	J/mol×K	517.04	Joback Method
cpg	225.35	J/mol×K	558.53	Joback Method
cpg	236.54	J/mol×K	600.01	Joback Method
cpg	246.90	J/mol×K	641.50	Joback Method
cpg	256.50	J/mol×K	682.99	Joback Method
cpg	265.37	J/mol×K	724.48	Joback Method
dvisc	0.0035890	Pa×s	248.13	Joback Method
dvisc	0.0018843	Pa×s	286.03	Joback Method

dvisc	0.0011503	Pa×s	323.94	Joback Method
dvisc	0.0007787	Pa×s	361.84	Joback Method
dvisc	0.0005676	Pa×s	399.74	Joback Method
dvisc	0.0004371	Pa×s	437.65	Joback Method
dvisc	0.0003509	Pa×s	475.55	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=R25320&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