Isopropylcyclobutane

Other names: Cyclobutane, isopropyl-
Inchi: InChI=1S/C7H14/c1-6(2)7-4-3-5-7/h6-7H,3-5H2,1-2H3
InchiKey: RFHQRRJFJJCQDJ-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC(C)C1CCC1
Mol. weight [g/mol]: 98.19
CAS: 872-56-0

Physical Properties

Property code	Value	Unit	Source
gf	54.27	kJ/mol	Joback Method
hf	-126.45	kJ/mol	Joback Method
hfus	6.40	kJ/mol	Joback Method
hvap	30.87	kJ/mol	Joback Method
ie	9.28 ± 0.05	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	690.90		NIST Webbook
rinpol	690.90		NIST Webbook
tb	365.85 ± 0.20	K	NIST Webbook
tb	365.70 ± 1.00	K	NIST Webbook
tc	560.61	K	Joback Method
tf	166.72 ± 0.20	K	NIST Webbook
tf	166.80 ± 0.40	K	NIST Webbook
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.51	J/mol×K	370.13	Joback Method
cpg	190.34	J/mol×K	401.88	Joback Method
cpg	204.42	J/mol×K	433.62	Joback Method

cpg	217.80	J/mol×K	465.37	Joback Method
cpg	230.50	J/mol×K	497.12	Joback Method
cpg	242.55	J/mol×K	528.86	Joback Method
cpg	253.98	J/mol×K	560.61	Joback Method
dvisc	0.0029826	Pa×s	168.07	Joback Method
dvisc	0.0014810	Pa×s	201.75	Joback Method
dvisc	0.0008984	Pa×s	235.42	Joback Method
dvisc	0.0006176	Pa×s	269.10	Joback Method
dvisc	0.0004615	Pa×s	302.78	Joback Method
dvisc	0.0003656	Pa×s	336.45	Joback Method
dvisc	0.0003021	Pa×s	370.13	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C872560&Units=SI

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
ie: Ionization energy
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