

Cyclopropane, 1-methyl-1-isopropenyl-

Inchi:	InChI=1S/C7H12/c1-6(2)7(3)4-5-7/h1,4-5H2,2-3H3
InchiKey:	PQMFTBQGLFFXOQ-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	C=C(C)C1(C)CC1
Mol. weight [g/mol]:	96.17
CAS:	3422-07-9

Physical Properties

Property code	Value	Unit	Source
gf	142.61	kJ/mol	Joback Method
hf	15.87	kJ/mol	Joback Method
hfus	3.13	kJ/mol	Joback Method
hvap	29.35	kJ/mol	Joback Method
ie	9.03	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	363.10	K	Joback Method
tc	557.69	K	Joback Method
tf	194.77	K	Joback Method
vc	0.364	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.70	J/molxK	363.10	Joback Method
cpg	178.02	J/molxK	395.53	Joback Method
cpg	191.17	J/molxK	427.96	Joback Method
cpg	203.25	J/molxK	460.40	Joback Method
cpg	214.37	J/molxK	492.83	Joback Method
cpg	224.62	J/molxK	525.26	Joback Method
cpg	234.09	J/molxK	557.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3422079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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