

Cyclopropane, 1-methyl-1-(1-methylethyl)

Inchi:	InChI=1S/C9H18/c1-8(2)9(3)6-4-5-7-9/h8H,4-7H2,1-3H3
InchiKey:	XFMQGDWBNOQLEG-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC(C)C1(C)CCCC1
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	53.52	kJ/mol	Joback Method
hf	-158.65	kJ/mol	Joback Method
hfus	3.18	kJ/mol	Joback Method
hvap	34.35	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mvol	126.810	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	646.00		NIST Webbook
rinpol	646.00		NIST Webbook
tb	420.40	K	Joback Method
tc	624.93	K	Joback Method
tf	210.99	K	Joback Method
vc	0.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.81	J/mol×K	420.40	Joback Method
cpg	275.53	J/mol×K	454.49	Joback Method
cpg	293.00	J/mol×K	488.58	Joback Method
cpg	309.32	J/mol×K	522.67	Joback Method
cpg	324.60	J/mol×K	556.76	Joback Method
cpg	338.93	J/mol×K	590.85	Joback Method
cpg	352.42	J/mol×K	624.93	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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol513.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143514&Units=SI

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
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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