

1,1-DIMETHYLCYCLOBUTANE

Inchi:	InChI=1S/C6H12/c1-6(2)4-3-5-6/h3-5H2,1-2H3
InchiKey:	OFZYBEBWCZBCPM-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	CC1(C)CCC1
Mol. weight [g/mol]:	84.16

Physical Properties

Property code	Value	Unit	Source
gf	42.80	kJ/mol	Joback Method
hf	-85.29	kJ/mol	Joback Method
hfus	1.03	kJ/mol	Joback Method
hvap	27.88	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.196		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	347.93	K	Joback Method
tc	543.37	K	Joback Method
tf	195.70	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.32	J/molxK	347.93	Joback Method
cpg	152.73	J/molxK	380.50	Joback Method
cpg	166.04	J/molxK	413.08	Joback Method
cpg	178.32	J/molxK	445.65	Joback Method
cpg	189.68	J/molxK	478.22	Joback Method
cpg	200.20	J/molxK	510.79	Joback Method
cpg	209.97	J/molxK	543.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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/mol464.mol

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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