

Cyclobutane, (1-methylethylidene)-

Inchi:	InChI=1S/C7H12/c1-6(2)7-4-3-5-7/h3-5H2,1-2H3
InchiKey:	UEVOQCSGNIHNLH-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC(C)=C1CCC1
Mol. weight [g/mol]:	96.17
CAS:	1528-22-9

Physical Properties

Property code	Value	Unit	Source
gf	101.33	kJ/mol	Joback Method
hf	-34.59	kJ/mol	Joback Method
hfus	7.86	kJ/mol	Joback Method
hvap	32.44	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.507		Crippen Method
mvol	94.330	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
tb	380.41 ± 0.30	K	NIST Webbook
tc	580.04	K	Joback Method
tf	214.82 ± 0.20	K	NIST Webbook
vc	0.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.82	J/mol×K	381.76	Joback Method
cpg	177.95	J/mol×K	414.81	Joback Method
cpg	190.34	J/mol×K	447.85	Joback Method
cpg	202.01	J/mol×K	480.90	Joback Method
cpg	213.01	J/mol×K	513.95	Joback Method
cpg	223.38	J/mol×K	546.99	Joback Method
cpg	233.15	J/mol×K	580.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1528229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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