

Cyclobutene, 3,3-dimethyl-

Inchi:	InChI=1S/C6H10/c1-6(2)4-3-5-6/h3-4H,5H2,1-2H3
InchiKey:	ZLUNIANKFULIMZ-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	CC1(C)C=CC1
Mol. weight [g/mol]:	82.14
CAS:	16327-38-1

Physical Properties

Property code	Value	Unit	Source
gf	72.76	kJ/mol	Joback Method
hf	-27.51	kJ/mol	Joback Method
hfus	2.25	kJ/mol	Joback Method
hvap	28.18	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.973		Crippen Method
mcvol	80.240	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
tb	347.09	K	Joback Method
tc	544.64	K	Joback Method
tf	196.46	K	Joback Method
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.99	J/mol×K	347.09	Joback Method
cpg	141.09	J/mol×K	380.01	Joback Method
cpg	153.10	J/mol×K	412.94	Joback Method
cpg	164.11	J/mol×K	445.86	Joback Method
cpg	174.21	J/mol×K	478.79	Joback Method
cpg	183.50	J/mol×K	511.71	Joback Method
cpg	192.07	J/mol×K	544.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16327381&Units=SI
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

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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