

Cyclobutane, 1,3-dimethyl

Inchi:	InChI=1S/C6H12/c1-5-3-6(2)4-5/h5-6H,3-4H2,1-2H3
InchiKey:	WKHRDGKOKYBNDZ-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	CC1CC(C)C1
Mol. weight [g/mol]:	84.16
CAS:	7411-24-7

Physical Properties

Property code	Value	Unit	Source
gf	40.58	kJ/mol	Joback Method
hf	-120.87	kJ/mol	Joback Method
hfus	8.40	kJ/mol	Joback Method
hvap	28.73	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	2.052		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	343.02	K	Joback Method
tc	528.71	K	Joback Method
tf	167.56	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.78	J/molxK	343.02	Joback Method
cpg	151.96	J/molxK	373.97	Joback Method
cpg	164.56	J/molxK	404.92	Joback Method
cpg	176.58	J/molxK	435.86	Joback Method
cpg	188.05	J/molxK	466.81	Joback Method
cpg	198.98	J/molxK	497.76	Joback Method
cpg	209.40	J/molxK	528.71	Joback Method
dvisc	0.0006361	Paxs	167.56	Joback Method
dvisc	0.0004767	Paxs	196.80	Joback Method

dvisc	0.0003849	Paxs	226.05	Joback Method
dvisc	0.0003264	Paxs	255.29	Joback Method
dvisc	0.0002864	Paxs	284.53	Joback Method
dvisc	0.0002574	Paxs	313.78	Joback Method
dvisc	0.0002357	Paxs	343.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7411247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	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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