

1,4-Cyclohexadiene, 1,2-dimethyl-

Other names:	1,2-Dimethyl-1,4-cyclohexadiene
Inchi:	InChI=1S/C8H12/c1-7-5-3-4-6-8(7)2/h3-4H,5-6H2,1-2H3
InchiKey:	QBSFOUVYWBKBF-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	CC1=C(C)CC=CC1
Mol. weight [g/mol]:	108.18
CAS:	17351-28-9

Physical Properties

Property code	Value	Unit	Source
gf	89.30	kJ/mol	Joback Method
hf	-41.17	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	36.05	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	414.94	K	Joback Method
tc	623.73	K	Joback Method
tf	218.10	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.88	J/molxK	414.94	Joback Method
cpg	251.30	J/molxK	588.93	Joback Method
cpg	240.29	J/molxK	554.14	Joback Method
cpg	228.67	J/molxK	519.34	Joback Method
cpg	216.40	J/molxK	484.54	Joback Method
cpg	203.48	J/molxK	449.74	Joback Method
cpg	261.72	J/molxK	623.73	Joback Method
dvisc	0.0002292	Paxs	414.94	Joback Method

dvisc	0.0002903	Paxs	382.13	Joback Method
dvisc	0.0003843	Paxs	349.33	Joback Method
dvisc	0.0005393	Paxs	316.52	Joback Method
dvisc	0.0008183	Paxs	283.71	Joback Method
dvisc	0.0013849	Paxs	250.91	Joback Method
dvisc	0.0027458	Paxs	218.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17351289&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

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
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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