

Cyclopentene, 1,5-dimethyl-

Other names:	1,2-DIMETHYL-2-CYCLOPENTENE 1,5-DIMETHYLCYCLOPENTENE 2,3-DIMETHYLCYCLOPENTENE
Inchi:	InChI=1S/C7H12/c1-6-4-3-5-7(6)2/h4,7H,3,5H2,1-2H3
InchiKey:	RIICRLQIUAAOOE-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC1=CCCC1C
Mol. weight [g/mol]:	96.17
CAS:	16491-15-9

Physical Properties

Property code	Value	Unit	Source
gf	64.94	kJ/mol	Joback Method
hf	-81.02	kJ/mol	Joback Method
hfus	8.65	kJ/mol	Joback Method
hvap	32.39	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	697.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	697.00		NIST Webbook
tb	375.20	K	NIST Webbook
tb	365.70 ± 3.00	K	NIST Webbook
tb	368.90 ± 3.00	K	NIST Webbook
tb	368.64	K	KDB
tc	576.72	K	Joback Method
tf	154.70 ± 0.50	K	NIST Webbook
vc	0.354	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	164.57	J/molxK	378.98	Joback Method
cpg	178.00	J/molxK	411.94	Joback Method
cpg	190.80	J/molxK	444.89	Joback Method
cpg	202.99	J/molxK	477.85	Joback Method
cpg	214.58	J/molxK	510.81	Joback Method
cpg	225.59	J/molxK	543.77	Joback Method
cpg	236.05	J/molxK	576.72	Joback Method
dvisc	0.0016528	Paxs	192.83	Joback Method
dvisc	0.0009756	Paxs	223.85	Joback Method
dvisc	0.0006547	Paxs	254.88	Joback Method
dvisc	0.0004791	Paxs	285.90	Joback Method
dvisc	0.0003727	Paxs	316.93	Joback Method
dvisc	0.0003032	Paxs	347.96	Joback Method
dvisc	0.0002552	Paxs	378.98	Joback Method
hvapt	37.10	kJ/mol	348.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38619e+01
Coeff. B	-2.98264e+03
Coeff. C	-5.25280e+01
Temperature range (K), min.	272.26
Temperature range (K), max.	401.36

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=622
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16491159&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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