

Cyclopentene, 1,2-dimethyl-

Other names:	1,2-Dimethylcyclopentene 1,2-dimethyl-1-cyclopentene
Inchi:	InChI=1S/C7H12/c1-6-4-3-5-7(6)2/h3-5H2,1-2H3
InchiKey:	SZZWLAZADBEDQP-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC1=C(C)CCC1
Mol. weight [g/mol]:	96.17
CAS:	765-47-9

Physical Properties

Property code	Value	Unit	Source
affp	822.60	kJ/mol	NIST Webbook
basg	791.90	kJ/mol	NIST Webbook
gf	63.02	kJ/mol	Joback Method
hf	-41.40	kJ/mol	NIST Webbook
hfus	7.19	kJ/mol	Joback Method
hvap	33.36	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.507		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	743.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	710.00		NIST Webbook
tb	366.40 ± 1.00	K	NIST Webbook
tb	378.30 ± 2.00	K	NIST Webbook
tb	378.18 ± 0.40	K	NIST Webbook
tb	376.70 ± 3.00	K	NIST Webbook
tb	378.95 ± 0.30	K	NIST Webbook
tb	375.70 ± 2.00	K	NIST Webbook
tb	376.00 ± 6.00	K	NIST Webbook
tb	377.80 ± 2.00	K	NIST Webbook
tb	379.00	K	NIST Webbook

tb	378.18	K	KDB
tc	588.63	K	Joback Method
tf	182.75 ± 0.50	K	NIST Webbook
vc	0.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.33	J/mol×K	588.63	Joback Method
cpg	223.50	J/mol×K	555.30	Joback Method
cpg	213.15	J/mol×K	521.96	Joback Method
cpg	202.24	J/mol×K	488.63	Joback Method
cpg	190.78	J/mol×K	455.30	Joback Method
cpg	178.72	J/mol×K	421.96	Joback Method
cpg	166.06	J/mol×K	388.63	Joback Method
dvisc	0.0020148	Paxs	209.59	Joback Method
dvisc	0.0002610	Paxs	388.63	Joback Method
dvisc	0.0003184	Paxs	358.79	Joback Method
dvisc	0.0004028	Paxs	328.95	Joback Method
dvisc	0.0005340	Paxs	299.11	Joback Method
dvisc	0.0007537	Paxs	269.27	Joback Method
dvisc	0.0011590	Paxs	239.43	Joback Method
hvapt	36.40	kJ/mol	362.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41360e+01
Coeff. B	-3.07332e+03
Coeff. C	-5.30930e+01
Temperature range (K), min.	275.02
Temperature range (K), max.	401.36

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol619.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765479&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
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
h vap:	Enthalpy of vaporization at standard conditions
h vap t:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
p vap:	Vapor pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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