Cyclopentane, 1,3-dimethyl-

Other names: 1,3-Dimethylcyclopentane
Inchi: InChI=1S/C7H14/c1-6-3-4-7(2)5-6/h6-7H,3-5H2,1-2H3
InchiKey: XAZKFISIRYLAEE-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC1CCC(C)C1
Mol. weight [g/mol]: 98.19
CAS: 2453-00-1

Physical Properties

Property code	Value	Unit	Source
chl	-4599.90	kJ/mol	NIST Webbook
gf	36.90	kJ/mol	Joback Method
hf	-147.67	kJ/mol	Joback Method
hfus	8.89	kJ/mol	Joback Method
hvap	31.12	kJ/mol	Joback Method
ie	9.56 ± 0.05	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	681.00		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	690.00		NIST Webbook
tb	366.00 ± 6.00	K	NIST Webbook
tb	364.20 ± 0.50	K	NIST Webbook
tb	364.33 ± 0.80	K	NIST Webbook
tc	563.52	K	Joback Method
tf	132.60 ± 0.50	K	NIST Webbook
tf	132.60 ± 2.00	K	NIST Webbook
tf	136.50 ± 3.00	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.95	J/mol×K	370.17	Joback Method
cpg	189.42	J/mol×K	402.40	Joback Method
cpg	204.20	J/mol×K	434.62	Joback Method
cpg	218.32	J/mol×K	466.85	Joback Method
cpg	231.80	J/mol×K	499.07	Joback Method
cpg	244.64	J/mol×K	531.30	Joback Method
cpg	256.86	J/mol×K	563.52	Joback Method
dvisc	0.0017720	Pa×s	175.31	Joback Method
dvisc	0.0010080	Pa×s	207.79	Joback Method
dvisc	0.0006678	Pa×s	240.26	Joback Method
dvisc	0.0004881	Pa×s	272.74	Joback Method
dvisc	0.0003813	Pa×s	305.22	Joback Method
dvisc	0.0003124	Pa×s	337.69	Joback Method
dvisc	0.0002650	Pa×s	370.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34613e+01
Coeff. B	-2.84463e+03
Coeff. C	-4.26480e+01
Temperature range (K), min.	258.58
Temperature range (K), max.	391.69

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2453001&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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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