Cyclopentane, 1,1,2-trimethyl-

Other names:	1,1,2-TRIMETHYLCYCLOPENTANE
	CAMPHOCEAN
Inchi:	InChI=1S/C8H16/c1-7-5-4-6-8(7,2)3/h7H,4-6H2,1-3H3
InchiKey:	WINCSBAYCULVDU-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC1CCCC1(C)C
Mol. weight [g/mol]:	112.21
CAS:	4259-00-1

Physical Properties

Property code	Value	Unit	Source
gf	39.83	kJ/mol	Joback Method
hf	-153.07	kJ/mol	Joback Method
hfus	5.18	kJ/mol	Joback Method
hvap	37.20	kJ/mol	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	749.00		NIST Webbook
rinpol	777.90		NIST Webbook
rinpol	758.90		NIST Webbook
rinpol	761.40		NIST Webbook
rinpol	763.80		NIST Webbook
rinpol	766.30		NIST Webbook
rinpol	763.40		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	764.40		NIST Webbook
rinpol	764.80		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	761.00		NIST Webbook

rinpol	768.40	NIST Webbook
rinpol	768.40	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	760.00	NIST Webbook
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rinpol	764.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	760.30	NIST Webbook
rinpol	761.10	NIST Webbook
rinpol	759.70	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	772.60	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	762.00	NIST Webbook
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rinpol	729.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	768.60		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook
tb	386.87 ± 0.02	K	NIST Webbook
tb	386.85 ± 0.30	K	NIST Webbook
tb	386.88	K	KDB
tb	386.90 ± 0.20	K	NIST Webbook
tc	594.34	K	Joback Method
tf	251.20 ± 0.40	K	NIST Webbook
tf	251.48 ± 0.15	K	NIST Webbook
tf	251.20 ± 0.40	K	NIST Webbook
tf	251.51 ± 0.05	K	NIST Webbook
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.45	J/mol×K	393.29	Joback Method
cpg	232.08	J/mol×K	426.80	Joback Method
cpg	248.56	J/mol×K	460.31	Joback Method
cpg	263.98	J/mol×K	493.81	Joback Method
cpg	278.43	J/mol×K	527.32	Joback Method
cpg	292.00	J/mol×K	560.83	Joback Method
cpg	304.76	J/mol×K	594.34	Joback Method
hvapt	36.30	kJ/mol	324.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38657e+01
Coeff. B	-3.11289e+03
Coeff. C	-5.02760e+01
Temperature range (K), min.	251.51
Temperature range (K), max.	414.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.48795e+01
Coeff. B	-7.22220e+03
Coeff. C	-1.05427e+01
Coeff. D	8.15777e-06
Temperature range (K), min.	309.15
Temperature range (K), max.	389.15

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=487

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4259001&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=487

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

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
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