Cyclopropane, 1,1,2-trimethyl-

Other names: 1,1,2-Trimethylcyclopropane
Inchi: InChI=1S/C6H12/c1-5-4-6(5,2)3/h5H,4H2,1-3H3
InchiKey: BXIIJPAVISPOGI-UHFFFAOYSA-N
Formula: C6H12
SMILES: CC1CC1(C)C
Mol. weight [g/mol]: 84.16
CAS: 4127-45-1

Physical Properties

Property code	Value	Unit	Source
chl	-3979.90 ± 0.75	kJ/mol	NIST Webbook
gf	47.19	kJ/mol	Joback Method
hf	-99.47	kJ/mol	Joback Method
hfl	-96.19 ± 0.84	kJ/mol	NIST Webbook
hfus	4.20	kJ/mol	Joback Method
hvap	27.40	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
log10ws	-1.75		Crippen Method
logp	2.052		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpol	552.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	549.90		NIST Webbook
rinpol	549.90		NIST Webbook
rinpol	548.50		NIST Webbook
rinpol	550.00		NIST Webbook

rinpol	549.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	548.00		NIST Webbook
tb	325.75 ± 1.00	K	NIST Webbook
tb	330.15 ± 3.00	K	NIST Webbook
tb	325.70 ± 0.30	K	NIST Webbook
tb	325.70 ± 0.20	K	NIST Webbook
tb	325.64 ± 0.20	K	NIST Webbook
tb	325.70 ± 0.30	K	NIST Webbook
tb	325.71 ± 0.20	K	NIST Webbook
tb	325.70 ± 0.20	K	NIST Webbook
tb	325.80 ± 0.60	K	NIST Webbook
tb	326.15 ± 2.00	K	NIST Webbook
tc	525.10	K	Joback Method
tf	134.86 ± 0.30	K	NIST Webbook
tf	134.76 ± 0.30	K	NIST Webbook
tf	134.97 ± 0.05	K	NIST Webbook
tf	134.94 ± 0.08	K	NIST Webbook
tf	134.98 ± 0.20	K	NIST Webbook
tf	134.98 ± 0.20	K	NIST Webbook
tf	134.88 ± 0.20	K	NIST Webbook
tf	134.86 ± 0.25	K	NIST Webbook
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.60	J/mol×K	338.99	Joback Method
cpg	154.35	J/mol×K	370.01	Joback Method
cpg	167.09	J/mol×K	401.03	Joback Method
cpg	178.89	J/mol×K	432.04	Joback Method
cpg	189.85	J/mol×K	463.06	Joback Method
cpg	200.02	J/mol×K	494.08	Joback Method
cpg	209.50	J/mol×K	525.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51914e+01
Coeff. B	-3.11203e+03
Coeff. C	-3.16640e+01
Temperature range (K), min.	240.47
Temperature range (K), max.	346.65

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=460
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4127451&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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