Methylcyclopropane

Inchi: InChI=1S/C4H8/c1-4-2-3-4/h4H,2-3H2,1H3
InchiKey: VNXBKJFUJUWOCW-UHFFFAOYSA-N
Formula: C4H8
SMILES: CC1CC1
Mol. weight [g/mol]: 56.11
CAS: 594-11-6

Physical Properties

Property code	Value	Unit	Source
chl	-2719.10 ± 0.59	kJ/mol	NIST Webbook
gf	43.55	kJ/mol	Joback Method
hf	-53.09	kJ/mol	Joback Method
hfl	1.70 ± 0.67	kJ/mol	NIST Webbook
hfus	4.25	kJ/mol	Joback Method
hvap	24.41	kJ/mol	Joback Method
ie	9.46	eV	NIST Webbook
ie	9.30 ± 0.05	eV	NIST Webbook
ie	9.90 ± 0.20	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.416		Crippen Method
mcvol	56.360	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
rinpol	415.00		NIST Webbook
rinpol	414.50		NIST Webbook
tb	273.88 ± 0.20	K	NIST Webbook
tb	277.65 ± 3.00	K	NIST Webbook
tb	277.65 ± 3.00	K	NIST Webbook
tb	273.85 ± 0.30	K	NIST Webbook
tb	273.88 ± 0.20	K	NIST Webbook
tb	273.85 ± 0.30	K	NIST Webbook
tc	475.09	K	Joback Method
tf	95.91 ± 0.05	K	NIST Webbook
tf	96.10 ± 0.10	K	NIST Webbook
tf	96.12 ± 0.10	K	NIST Webbook
tf	95.64 ± 0.20	K	NIST Webbook
tf	95.83 ± 0.10	K	NIST Webbook
tf	96.12 ± 0.10	K	NIST Webbook

tf	95.99 ± 0.10	K	NIST Webbook
tf	95.85 ± 0.20	K	NIST Webbook
tf	95.85 ± 0.20	K	NIST Webbook
tf	95.91 ± 0.03	K	NIST Webbook
tt	95.64 ± 0.20	K	NIST Webbook
vc	0.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.16	J/mol×K	475.09	Joback Method
cpg	117.06	J/mol×K	445.52	Joback Method
cpg	109.56	J/mol×K	415.95	Joback Method
cpg	101.64	J/mol×K	386.37	Joback Method
cpg	93.26	J/mol×K	356.80	Joback Method
cpg	84.41	J/mol×K	327.23	Joback Method
cpg	75.07	J/mol×K	297.66	Joback Method
dvisc	0.0002982	Pa×s	152.78	Joback Method
dvisc	0.0001728	Pa×s	297.66	Joback Method
dvisc	0.0001818	Pa×s	273.51	Joback Method
dvisc	0.0001932	Pa×s	249.37	Joback Method
dvisc	0.0002079	Pa×s	225.22	Joback Method
dvisc	0.0002278	Pa×s	201.07	Joback Method
dvisc	0.0002559	Pa×s	176.93	Joback Method
hvapt	24.80	kJ/mol	227.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37558e+01
Coeff. B	-2.15673e+03
Coeff. C	-3.89700e+01
Temperature range (K), min.	199.10
Temperature range (K), max.	294.37

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594116&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol447.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfl:	Liquid phase 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
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
tt:	Triple Point Temperature
vc:	Critical Volume