Cyclohexane, methylene-

Other names: 1-Methylenecyclohexane
Methylenecyclohexane
Inchi: InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h1-6H2
InchiKey: YULMNMJFAZWLLN-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=C1CCCCC1
Mol. weight [g/mol]: 96.17
CAS: 1192-37-6

Physical Properties

Property code	Value	Unit	Source
chl	-4412.40	kJ/mol	NIST Webbook
gf	93.30	kJ/mol	Joback Method
hf	-28.91	kJ/mol	Joback Method
hfus	3.49	kJ/mol	Joback Method
hvap	36.10 ± 0.30	kJ/mol	NIST Webbook
hvap	36.10 ± 0.30	kJ/mol	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.13	eV	NIST Webbook
ie	9.12 ± 0.02	eV	NIST Webbook
ie	9.08 ± 0.01	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	9.13	eV	NIST Webbook
ie	9.04 ± 0.03	eV	NIST Webbook
ie	8.97 ± 0.01	eV	NIST Webbook
ie	8.94	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	8.93 ± 0.01	eV	NIST Webbook
log10ws	-2.50		Crippen Method
logp	2.507		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	736.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	741.70		NIST Webbook

rinpol	731.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	737.50		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	750.80		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	754.10		NIST Webbook
rinpol	759.30		NIST Webbook
rinpol	737.80		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	745.50		NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tb	376.11 ± 0.20	K	NIST Webbook
tb	378.15 ± 6.00	K	NIST Webbook
tb	375.70 ± 0.70	K	NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tb	375.40 ± 4.00	K	NIST Webbook
tb	376.00 ± 4.00	K	NIST Webbook
tb	382.00 ± 5.00	K	NIST Webbook
tb	371.00 ± 1.00	K	NIST Webbook
tb	375.10 ± 2.00	K	NIST Webbook
tb	376.50 ± 1.00	K	NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tb	375.00 ± 3.00	K	NIST Webbook
tb	378.00 ± 6.00	K	NIST Webbook
tb	377.00 ± 5.00	K	NIST Webbook
tb	375.70	K	NIST Webbook
tb	379.00 ± 5.00	K	NIST Webbook
tb	379.00 ± 4.00	K	NIST Webbook
tb	376.17 ± 0.05	K	NIST Webbook
tb	379.00 ± 4.00	K	NIST Webbook

tc	588.02	K	Joback Method
tf	168.43 ± 0.03	K	NIST Webbook
tf	168.44 ± 0.02	K	NIST Webbook
tf	166.50 ± 0.50	K	NIST Webbook
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.60	J/mol×K	588.02	Joback Method
cpg	225.63	J/mol×K	553.84	Joback Method
cpg	214.03	J/mol×K	519.66	Joback Method
cpg	201.79	J/mol×K	485.48	Joback Method
cpg	188.89	J/mol×K	451.30	Joback Method
cpg	175.31	J/mol×K	417.12	Joback Method
cpg	161.02	J/mol×K	382.94	Joback Method
cpl	177.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0002894	Pa×s	382.94	Joback Method
dvisc	0.0003823	Pa×s	351.44	Joback Method
dvisc	0.0005334	Pa×s	319.94	Joback Method
dvisc	0.0008004	Pa×s	288.44	Joback Method
dvisc	0.0013267	Pa×s	256.95	Joback Method
dvisc	0.0025327	Pa×s	225.45	Joback Method
dvisc	0.0059647	Pa×s	193.95	Joback Method
hvapt	34.40	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37327e+01
Coeff. B	-2.91341e+03
Coeff. C	-5.60000e+01
Temperature range (K), min.	272.69
Temperature range (K), max.	401.96

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192376&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
vc:	Critical Volume