Cyclobutane, ethyl-

Other names: Ethylcyclobutane
Inchi: InChI=1S/C6H12/c1-2-6-4-3-5-6/h6H,2-5H2,1H3
InchiKey: NEZRFXZYPAIZAD-UHFFFAOYSA-N
Formula: C6H12
SMILES: CCC1CCC1
Mol. weight [g/mol]: 84.16
CAS: 4806-61-5

Physical Properties

Property code	Value	Unit	Source
chl	-4017.10 ± 0.67	kJ/mol	NIST Webbook
gf	48.29	kJ/mol	Joback Method
hf	-26.30 ± 1.10	kJ/mol	NIST Webbook
hf	-27.70 ± 0.70	kJ/mol	NIST Webbook
hfl	-58.95 ± 0.75	kJ/mol	NIST Webbook
hfus	7.33	kJ/mol	Joback Method
hvap	33.00 ± 0.80	kJ/mol	NIST Webbook
hvap	31.24 ± 0.03	kJ/mol	NIST Webbook
hvap	31.42	kJ/mol	NIST Webbook
hvap	32.60 ± 0.80	kJ/mol	NIST Webbook
hvap	31.20 ± 0.20	kJ/mol	NIST Webbook
hvap	32.70	kJ/mol	NIST Webbook
ie	9.38 ± 0.05	eV	NIST Webbook
log10ws	-1.99		Crippen Method
logp	2.196		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	623.00		NIST Webbook
rinpol	627.30		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	619.37		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	627.30		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	623.00		NIST Webbook

rinpol	622.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	623.00		NIST Webbook
ripol	692.00		NIST Webbook
tb	347.69	K	Joback Method
tc	534.16	K	Joback Method
tf	171.80	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.57	J/mol×K	347.69	Joback Method
cpg	151.63	J/mol×K	378.77	Joback Method
cpg	164.06	J/mol×K	409.85	Joback Method
cpg	175.88	J/mol×K	440.92	Joback Method
cpg	187.10	J/mol×K	472.00	Joback Method
cpg	197.76	J/mol×K	503.08	Joback Method
cpg	207.88	J/mol×K	534.16	Joback Method
dvisc	0.0015104	Pa×s	171.80	Joback Method
dvisc	0.0009289	Pa×s	201.12	Joback Method
dvisc	0.0006465	Pa×s	230.43	Joback Method
dvisc	0.0004883	Pa×s	259.75	Joback Method
dvisc	0.0003904	Pa×s	289.06	Joback Method
dvisc	0.0003253	Pa×s	318.38	Joback Method
dvisc	0.0002795	Pa×s	347.69	Joback Method
hvapt	28.67	kJ/mol	343.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47747e+01
Coeff. B	-3.11889e+03
Coeff. C	-3.67120e+01
Temperature range (K), min.	252.00
Temperature range (K), max.	366.29

Sources

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/mol463.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4806615&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.