1-Ethylcyclopentene

Other names:	1-ETHYL-1-CYCLOPENTENE
	1-Ethylcyclopentene-1
	Cyclopentene, 1-ethyl-
	ETHYLCYCLOPENTENE
Inchi:	InChI=1S/C7H12/c1-2-7-5-3-4-6-7/h5H,2-4,6H2,1H3
InchiKey:	QYYQTLLGVAPKPN-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CCC1=CCCC1
Mol. weight [g/mol]:	96.17
CAS:	2146-38-5

Physical Properties

Property code	Value	Unit	Source
chl	-4411.27 ± 0.79	kJ/mol	NIST Webbook
gf	72.65	kJ/mol	Joback Method
hf	-25.00	kJ/mol	NIST Webbook
hf	-19.90 ± 0.90	kJ/mol	NIST Webbook
hfl	-58.37 ± 0.88	kJ/mol	NIST Webbook
hfus	7.58	kJ/mol	Joback Method
hvap	38.50 ± 0.30	kJ/mol	NIST Webbook
hvap	38.50 ± 0.30	kJ/mol	NIST Webbook
ie	8.53 ± 0.01	eV	NIST Webbook
log10ws	-2.50		Crippen Method
logp	2.507		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	748.40		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	750.90		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	775.00		NIST Webbook

rinpol	779.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	746.10		NIST Webbook
rinpol	747.40		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	747.40		NIST Webbook
ripol	880.50		NIST Webbook
ripol	891.00		NIST Webbook
ripol	880.50		NIST Webbook
ripol	891.10		NIST Webbook
ripol	880.50		NIST Webbook
ripol	891.10		NIST Webbook
ripol	891.00		NIST Webbook
ripol	886.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	891.00		NIST Webbook
ripol	885.90		NIST Webbook
ripol	885.90		NIST Webbook
tb	379.50	K	NIST Webbook
tb	379.90 ± 2.00	K	NIST Webbook
tb	376.15 ± 0.50	K	NIST Webbook
tb	382.00 ± 4.00	K	NIST Webbook
tb	379.35 ± 0.30	K	NIST Webbook
tb	379.48 ± 0.30	K	NIST Webbook

tb	377.00 ± 3.00	K	NIST Webbook
tb	377.00 ± 3.00	K	NIST Webbook
tb	380.00 ± 3.00	K	NIST Webbook
tb	379.70 ± 3.00	K	NIST Webbook
tb	378.00 ± 2.00	K	NIST Webbook
tb	379.50 ± 0.30	K	NIST Webbook
tb	379.70 ± 0.50	K	NIST Webbook
tb	379.70 ± 0.40	K	NIST Webbook
tb	380.00 ± 1.00	K	NIST Webbook
tb	381.00 ± 3.00	K	NIST Webbook
tb	380.50 ± 1.00	K	NIST Webbook
tc	582.00	K	Joback Method
tf	154.35 ± 0.30	K	NIST Webbook
tf	149.80 ± 0.50	K	NIST Webbook
vc	0.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.17	J/mol×K	383.65	Joback Method
cpg	177.41	J/mol×K	416.71	Joback Method
cpg	189.97	J/mol×K	449.77	Joback Method
cpg	201.88	J/mol×K	482.82	Joback Method
cpg	213.16	J/mol×K	515.88	Joback Method
cpg	223.84	J/mol×K	548.94	Joback Method
cpg	233.94	J/mol×K	582.00	Joback Method
cpl	188.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0031534	Pa×s	197.07	Joback Method
dvisc	0.0015999	Pa×s	228.17	Joback Method
dvisc	0.0009552	Pa×s	259.26	Joback Method
dvisc	0.0006369	Pa×s	290.36	Joback Method
dvisc	0.0004593	Pa×s	321.46	Joback Method
dvisc	0.0003509	Pa×s	352.55	Joback Method
dvisc	0.0002801	Pa×s	383.65	Joback Method
hvapt	36.50	kJ/mol	363.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41400e+01
Coeff. B	-3.14169e+03
Coeff. C	-4.90480e+01
Temperature range (K), min.	275.85
Temperature range (K), max.	404.91

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2146385&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/mol616.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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