Cyclopentene, 3-ethyl-

Other names:	3-ETHYL-1-CYCLOPENTENE
	3-ETHYLCYCLOPENTENE
	3-Ethylcyclopentene-1
Inchi:	InChI=1S/C7H12/c1-2-7-5-3-4-6-7/h3,5,7H,2,4,6H2,1H3
InchiKey:	HICUGGYRYZOXJI-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CCC1C=CCC1
Mol. weight [g/mol]:	96.17
CAS:	694-35-9

Physical Properties

Property code	Value	Unit	Source
gf	74.57	kJ/mol	Joback Method
hf	-12.40	kJ/mol	NIST Webbook
hfus	9.04	kJ/mol	Joback Method
hvap	31.73	kJ/mol	Joback Method
ie	8.88 ± 0.01	eV	NIST Webbook
ie	8.91 ± 0.05	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	714.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	712.90		NIST Webbook
rinpol	715.30		NIST Webbook
rinpol	718.70		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	716.00		NIST Webbook

rinpol	720.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	716.60		NIST Webbook
rinpol	712.40		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	716.00		NIST Webbook
ripol	842.80		NIST Webbook
ripol	849.20		NIST Webbook
ripol	842.80		NIST Webbook
ripol	836.50		NIST Webbook
ripol	849.20		NIST Webbook
ripol	836.50		NIST Webbook
ripol	843.00		NIST Webbook
ripol	836.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	849.00		NIST Webbook
tb	371.00	K	NIST Webbook
tb	370.92 ± 0.30	K	NIST Webbook
tb	371.20 ± 1.00	K	NIST Webbook
tb	371.30 ± 1.00	K	NIST Webbook
tb	369.00 ± 3.00	K	NIST Webbook
tb	370.96 ± 0.20	K	NIST Webbook
tb	370.95 ± 0.20	K	NIST Webbook
tb	370.96 ± 0.30	K	NIST Webbook
tb	370.96 ± 0.30	K	NIST Webbook
tb	370.00 ± 3.00	K	NIST Webbook
tc	570.05	K	Joback Method
tf	180.31	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	236.41	J/mol×K	570.05	Joback Method
cpg	225.67	J/mol×K	537.37	Joback Method
cpg	214.32	J/mol×K	504.70	Joback Method
cpg	202.34	J/mol×K	472.02	Joback Method
cpg	189.70	J/mol×K	439.35	Joback Method
cpg	176.38	J/mol×K	406.67	Joback Method
cpg	162.35	J/mol×K	374.00	Joback Method
dvisc	0.0026035	Pa×s	180.31	Joback Method
dvisc	0.0002734	Pa×s	374.00	Joback Method
dvisc	0.0003333	Pa×s	341.72	Joback Method
dvisc	0.0004235	Pa×s	309.44	Joback Method
dvisc	0.0005690	Pa×s	277.15	Joback Method
dvisc	0.0008265	Pa×s	244.87	Joback Method
dvisc	0.0013445	Pa×s	212.59	Joback Method
hvapt	36.50	kJ/mol	361.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40011e+01
Coeff. B	-2.98629e+03
Coeff. C	-5.27260e+01
Temperature range (K), min.	270.49
Temperature range (K), max.	396.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.37676e+01
Coeff. B	-7.43524e+03
Coeff. C	-1.18988e+01
Coeff. D	9.35331e-06
Temperature range (K), min.	323.15
Temperature range (K), max.	373.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=617
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694359&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=617
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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