Cyclopropene

Inchi: InChI=1S/C3H4/c1-2-3-1/h1-2H,3H2
InchiKey: OOXWYYGXTJLWHA-UHFFFAOYSA-N
Formula: C3H4
SMILES: C1=CC1
Mol. weight [g/mol]: 40.06
CAS: 2781-85-3

Physical Properties

Property code	Value	Unit	Source
affp	818.50	kJ/mol	NIST Webbook
basg	787.80	kJ/mol	NIST Webbook
chg	-2029.00 ± 3.00	kJ/mol	NIST Webbook
gf	72.80	kJ/mol	Joback Method
hf	45.67	kJ/mol	Joback Method
hfus	1.81	kJ/mol	Joback Method
hvap	22.79	kJ/mol	Joback Method
ie	9.64	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.67	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
ie	9.70 ± 0.10	eV	NIST Webbook
ie	9.70 ± 0.02	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
ie	9.67 ± 0.01	eV	NIST Webbook
ie	9.67 ± 0.01	eV	NIST Webbook
ie	9.82	eV	NIST Webbook
ie	9.67 ± 0.01	eV	NIST Webbook
log10ws	-0.83		Crippen Method
logp	0.946		Crippen Method
mcvol	37.970	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
tb	278.61	K	Joback Method
tc	457.65	K	Joback Method
tf	146.51	K	Joback Method
vc	0.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	38.20	J/mol×K	278.61	Joback Method
cpg	44.60	J/mol×K	308.45	Joback Method
cpg	50.54	J/mol×K	338.29	Joback Method
cpg	56.04	J/mol×K	368.13	Joback Method
cpg	61.14	J/mol×K	397.97	Joback Method
cpg	65.85	J/mol×K	427.81	Joback Method
cpg	70.21	J/mol×K	457.65	Joback Method
dvisc	0.0002886	Pa×s	146.51	Joback Method
dvisc	0.0002353	Pa×s	168.53	Joback Method
dvisc	0.0002011	Pa×s	190.54	Joback Method
dvisc	0.0001776	Pa×s	212.56	Joback Method
dvisc	0.0001605	Pa×s	234.58	Joback Method
dvisc	0.0001476	Pa×s	256.59	Joback Method
dvisc	0.0001375	Pa×s	278.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.99106e+02
Coeff. B	-1.15136e+06
Coeff. C	3.67034e+03
Temperature range (K), min.	179.15
Temperature range (K), max.	248.60

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2781853&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas 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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume