Spiropentane

Other names: Spiro[2.2]pentane
Inchi: InChI=1S/C5H8/c1-2-5(1)3-4-5/h1-4H2
InchiKey: OGNAOIGAPPSUMG-UHFFFAOYSA-N
Formula: C5H8
SMILES: C1CC12CC2
Mol. weight [g/mol]: 68.12
CAS: 157-40-4

Physical Properties

Property code	Value	Unit	Source
chg	-3258.00 ± 1.30	kJ/mol	NIST Webbook
chg	-3296.00 ± 0.71	kJ/mol	NIST Webbook
gf	127.04	kJ/mol	Joback Method
hf	185.10 ± 0.75	kJ/mol	NIST Webbook
hfus	-0.29	kJ/mol	Joback Method
hvap	27.70	kJ/mol	NIST Webbook
hvap	27.50 ± 0.10	kJ/mol	NIST Webbook
ie	9.37 ± 0.05	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.73	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
log10ws	-1.46		Crippen Method
logp	1.560		Crippen Method
mcvol	59.590	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
sl	193.68	J/mol×K	NIST Webbook
tb	303.18 ± 0.10	K	NIST Webbook
tb	312.18 ± 0.10	K	NIST Webbook
tb	312.10	K	NIST Webbook
tc	506.40	K	NIST Webbook
tf	166.10 ± 0.10	K	NIST Webbook
tf	166.10 ± 0.10	K	NIST Webbook
tt	166.14 ± 0.05	K	NIST Webbook
vc	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.69 ± 0.63	J/mol×K	283.16	NIST Webbook
cpg	282.21 ± 0.63	J/mol×K	298.16	NIST Webbook
cpg	286.35 ± 0.63	J/mol×K	312.14	NIST Webbook
cpl	134.52	J/mol×K	298.15	NIST Webbook
hfust	6.43	kJ/mol	166.10	NIST Webbook
hfust	6.43	kJ/mol	166.14	NIST Webbook
hfust	6.43	kJ/mol	166.10	NIST Webbook
hvapt	26.70 ± 0.10	kJ/mol	312.00	NIST Webbook
hvapt	26.76	kJ/mol	312.10	NIST Webbook
hvapt	26.75	kJ/mol	312.13	NIST Webbook
hvapt	28.60	kJ/mol	310.00	NIST Webbook
hvapt	28.30 ± 0.10	kJ/mol	283.00	NIST Webbook
sfust	38.72	J/mol×K	166.14	NIST Webbook
svapt	85.70	J/mol×K	312.13	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44024e+01
Coeff. B	-2.70023e+03
Coeff. C	-3.61160e+01
Temperature range (K), min.	227.42
Temperature range (K), max.	333.14

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C157404&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

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume