Cyclopropane, 1,1-diethyl-

Other names: 1,1-Diethylcyclopropane
Inchi: InChI=1S/C7H14/c1-3-7(4-2)5-6-7/h3-6H2,1-2H3
InchiKey: VUROAZUCSQPSOK-UHFFFAOYSA-N
Formula: C7H14
SMILES: CCC1(CC)CC1
Mol. weight [g/mol]: 98.19
CAS: 1003-19-6

Physical Properties

Property code	Value	Unit	Source
gf	63.32	kJ/mol	Joback Method
hf	-99.77	kJ/mol	Joback Method
hfus	5.72	kJ/mol	Joback Method
hvap	29.94	kJ/mol	Joback Method
ie	8.56 ± 0.05	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.587		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	673.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	672.80		NIST Webbook
rinpol	673.00		NIST Webbook
tb	361.82 ± 0.50	K	NIST Webbook
tb	361.79 ± 0.30	K	NIST Webbook
tb	361.79 ± 0.30	K	NIST Webbook
tb	361.81 ± 0.20	K	NIST Webbook
tb	361.82 ± 0.25	K	NIST Webbook
tc	552.93	K	Joback Method
tf	167.24 ± 0.20	K	NIST Webbook
tf	167.24 ± 0.20	K	NIST Webbook
tf	167.05 ± 0.20	K	NIST Webbook
tf	167.05 ± 0.25	K	NIST Webbook
tf	167.09 ± 0.30	K	NIST Webbook
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.76	J/mol×K	366.54	Joback Method
cpg	192.34	J/mol×K	397.60	Joback Method
cpg	205.86	J/mol×K	428.67	Joback Method
cpg	218.40	J/mol×K	459.73	Joback Method
cpg	230.05	J/mol×K	490.80	Joback Method
cpg	240.89	J/mol×K	521.86	Joback Method
cpg	251.00	J/mol×K	552.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52932e+01
Coeff. B	-3.41693e+03
Coeff. C	-4.17300e+01
Temperature range (K), min.	269.44
Temperature range (K), max.	384.05

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003196&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

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume