

Bicyclo[2.2.2]octane

Other names:	1,4-Endoethylenecyclohexane Cyclohexane, 1,4-endo-(1,2-ethanediyl)-
Inchi:	InChI=1S/C8H14/c1-2-8-5-3-7(1)4-6-8/h7-8H,1-6H2
InchiKey:	GPRLTFBKWDERLU-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	C1CC2CCC1CC2
Mol. weight [g/mol]:	110.20
CAS:	280-33-1

Physical Properties

Property code	Value	Unit	Source
chs	-5001.93 ± 0.88	kJ/mol	NIST Webbook
gf	113.78	kJ/mol	Joback Method
hf	-99.04 ± 0.96	kJ/mol	NIST Webbook
hfs	-147.10 ± 0.84	kJ/mol	NIST Webbook
hfus	8.55	kJ/mol	Joback Method
hsub	48.10	kJ/mol	NIST Webbook
hsub	47.70 ± 0.80	kJ/mol	NIST Webbook
hvap	33.57	kJ/mol	Joback Method
ie	9.45 ± 0.02	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
ie	9.43	eV	NIST Webbook
ie	9.47 ± 0.04	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.587		Crippen Method
mcvol	101.860	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	883.00		NIST Webbook
ripol	1007.00		NIST Webbook
sg	324.70 ± 2.50	J/mol×K	NIST Webbook
ss	209.95	J/mol×K	NIST Webbook
tb	404.46	K	Joback Method
tc	614.38	K	Joback Method
tf	443.00 ± 5.00	K	NIST Webbook
tt	447.48 ± 0.01	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.70	J/mol×K	404.46	Joback Method
cpg	217.06	J/mol×K	439.45	Joback Method
cpg	234.29	J/mol×K	474.43	Joback Method
cpg	250.43	J/mol×K	509.42	Joback Method
cpg	265.55	J/mol×K	544.41	Joback Method
cpg	279.71	J/mol×K	579.39	Joback Method
cpg	292.95	J/mol×K	614.38	Joback Method
cps	157.69	J/mol×K	298.15	NIST Webbook
dvisc	0.0004754	Pa×s	404.46	Joback Method
dvisc	0.0010230	Pa×s	241.38	Joback Method
dvisc	0.0013767	Pa×s	208.76	Joback Method
dvisc	0.0006827	Pa×s	306.61	Joback Method
dvisc	0.0005912	Pa×s	339.23	Joback Method
dvisc	0.0005251	Pa×s	371.84	Joback Method
dvisc	0.0008158	Pa×s	273.99	Joback Method
hfust	8.37	kJ/mol	447.50	NIST Webbook
hfust	4.60	kJ/mol	164.30	NIST Webbook
hfust	8.37	kJ/mol	447.50	NIST Webbook
hsubt	46.30 ± 0.80	kJ/mol	343.00	NIST Webbook
sfust	28.01	J/mol×K	164.30	NIST Webbook
sfust	18.70	J/mol×K	447.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.86803e+01
Coeff. B	-5.83153e+03
Temperature range (K), min.	317.06
Temperature range (K), max.	436.20

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=C280331&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/ci990307I

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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