Bicyclo[2.2.1]heptane

Other names:	1,4-Endomethylenecyclohexane
	Cyclohexane, 1,4-endo-methylene-
	Norbornylane
	Norcamphane
	Norfenchane
	Norsantane
Inchi:	InChI=1S/C7H12/c1-2-7-4-3-6(1)5-7/h6-7H,1-5H2
InchiKey:	UMRZSTCPUPJPOJ-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	C1CC2CCC1C2
Mol. weight [g/mol]:	96.17
CAS:	279-23-2

Physical Properties

Property code	Value	Unit	Source
chs	-4374.59 ± 0.97	kJ/mol	NIST Webbook
chs	-4367.50 ± 3.30	kJ/mol	NIST Webbook
chs	-4377.50 ± 2.20	kJ/mol	NIST Webbook
hf	-54.90 ± 1.10	kJ/mol	NIST Webbook
hf	-54.70 ± 4.70	kJ/mol	NIST Webbook
hf	-52.00	kJ/mol	NIST Webbook
hf	-52.00	kJ/mol	NIST Webbook
hfs	-95.00 ± 1.10	kJ/mol	NIST Webbook
hfs	-92.10 ± 2.70	kJ/mol	NIST Webbook
hfs	-92.10 ± 2.20	kJ/mol	NIST Webbook
hfs	-102.00 ± 3.30	kJ/mol	NIST Webbook
hfus	8.06	kJ/mol	Joback Method
hsub	47.30	kJ/mol	NIST Webbook
hsub	40.26 ± 0.32	kJ/mol	NIST Webbook
hsub	40.04 ± 0.18	kJ/mol	NIST Webbook
hsub	40.10	kJ/mol	NIST Webbook
hsub	40.00 ± 0.10	kJ/mol	NIST Webbook
hsub	40.30 ± 0.32	kJ/mol	NIST Webbook
hsub	40.40 ± 0.90	kJ/mol	NIST Webbook
hsub	40.10 ± 0.40	kJ/mol	NIST Webbook
hvap	36.25	kJ/mol	Cheméo Relay (1.0)
ie	9.77 ± 0.03	eV	NIST Webbook

ie	9.74	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	9.93 ± 0.02	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
logp	2.196		Crippen Method
mcvol	87.770	ml/mol	McGowan Method
rinpol	748.70		NIST Webbook
rinpol	745.20		NIST Webbook
rinpol	756.30		NIST Webbook
rinpol	756.30		NIST Webbook
rinpol	752.90		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	777.00		NIST Webbook
ripol	860.00		NIST Webbook
tb	381.00 ± 3.00	K	NIST Webbook
tf	360.90 ± 1.50	K	NIST Webbook
tf	360.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.30	J/mol×K	478.78	Joback Method
cpg	242.73	J/mol×K	580.24	Joback Method
cpg	231.09	J/mol×K	546.42	Joback Method
cpg	218.63	J/mol×K	512.60	Joback Method
cpg	159.53	J/mol×K	377.31	Joback Method
cpg	175.81	J/mol×K	411.13	Joback Method
cpg	191.05	J/mol×K	444.95	Joback Method
cps	151.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0006290	Pa×s	201.01	Joback Method
dvisc	0.0005714	Pa×s	230.39	Joback Method
dvisc	0.0005305	Pa×s	259.78	Joback Method
dvisc	0.0005001	Pa×s	289.16	Joback Method
dvisc	0.0004765	Pa×s	318.54	Joback Method
dvisc	0.0004578	Pa×s	347.93	Joback Method
dvisc	0.0004425	Pa×s	377.31	Joback Method

hfust	4.45	kJ/mol	360.80	NIST Webbook
hsubt	40.10 ± 0.84	kJ/mol	284.00	NIST Webbook
hsubt	40.00 ± 0.80	kJ/mol	305.00	NIST Webbook
hsubt	40.30 ± 0.40	kJ/mol	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54974e+01
Coeff. B	-3.70620e+03
Coeff. C	-3.77790e+01
Temperature range (K), min.	281.45
Temperature range (K), max.	401.63

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C279232&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point