Bicyclo[4.1.0]heptane

Other names: Norcarane
cis-Bicyclo[4.1.0]heptane
Inchi: InChI=1S/C7H12/c1-2-4-7-5-6(7)3-1/h6-7H,1-5H2
InchiKey: WPHGSKGZRAQSGP-UHFFFAOYSA-N
Formula: C7H12
SMILES: C1CCC2CC2C1
Mol. weight [g/mol]: 96.17
CAS: 286-08-8

Physical Properties

Property code	Value	Unit	Source
chl	-4433.00 ± 3.00	kJ/mol	NIST Webbook
chl	-4442.60 ± 1.70	kJ/mol	NIST Webbook
gf	117.46	kJ/mol	Joback Method
hf	2.00 ± 4.20	kJ/mol	NIST Webbook
hf	11.00	kJ/mol	NIST Webbook
hfl	-27.00 ± 1.70	kJ/mol	NIST Webbook
hfl	-36.00 ± 3.00	kJ/mol	NIST Webbook
hfus	8.06	kJ/mol	Joback Method
hvap	40.60 ± 0.20	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	38.10 ± 0.80	kJ/mol	NIST Webbook
ie	9.03 ± 0.02	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.196		Crippen Method
mcvol	87.770	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	797.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	797.00		NIST Webbook
tb	389.00 ± 2.00	K	NIST Webbook
tb	389.00 ± 2.00	K	NIST Webbook
tb	383.00	K	NIST Webbook
tb	389.00 ± 3.00	K	NIST Webbook
tb	389.00 ± 4.00	K	NIST Webbook

tc	580.24	K	Joback Method
tf	201.01	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	205.30	J/mol×K	478.78	Joback Method
cpg	218.63	J/mol×K	512.60	Joback Method
cpg	231.09	J/mol×K	546.42	Joback Method
cpg	242.73	J/mol×K	580.24	Joback Method
dvisc	0.0005714	Pa×s	230.39	Joback Method
dvisc	0.0006290	Pa×s	201.01	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
hvapt	38.00 ± 0.80	kJ/mol	341.50	NIST Webbook
hvapt	36.50	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41312e+01
Coeff. B	-3.23607e+03
Coeff. C	-4.94730e+01
Temperature range (K), min.	283.23
Temperature range (K), max.	416.38

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C286088&Units=SI

Legend

chl:	Standard liquid 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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume