Bicyclo[4.2.0]octane

Other names: cis-bicyclo[4.2.0]octane
Inchi: InChI=1S/C8H14/c1-2-4-8-6-5-7(8)3-1/h7-8H,1-6H2
InchiKey: RPZUBXWEQBPUJR-OCAPTIKFSA-N
Formula: C8H14
SMILES: C1CCC2CCC2C1
Mol. weight [g/mol]: 110.20
CAS: 278-30-8

Physical Properties

Property code	Value	Unit	Source
chl	-5081.00 ± 3.00	kJ/mol	NIST Webbook
hf	-26.00 ± 4.60	kJ/mol	NIST Webbook
hfl	-68.00 ± 3.00	kJ/mol	NIST Webbook
hfus	8.55	kJ/mol	Joback Method
hvap	42.00	kJ/mol	NIST Webbook
hvap	43.00 ± 1.00	kJ/mol	NIST Webbook
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-4.59		Cheméo Relay (1.0)
logp	2.587		Crippen Method
mcvol	101.860	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	409.90 ± 2.50	K	NIST Webbook
tc	637.51	K	Cheméo Relay (1.0)
tf	233.62	K	Cheméo Relay (1.0)

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
dvisc	0.0013767	Pa×s	208.76	Joback Method
dvisc	0.0010230	Pa×s	241.38	Joback Method
dvisc	0.0008158	Pa×s	273.99	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	0.0004754	Pa×s	404.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43834e+01
Coeff. B	-3.66003e+03
Coeff. C	-3.98930e+01
Temperature range (K), min.	298.00
Temperature range (K), max.	443.34

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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=C278308&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

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point