Bicyclo[5.1.0]octane

Inchi: InChI=1S/C8H14/c1-2-4-7-6-8(7)5-3-1/h7-8H,1-6H2
InchiKey: AKHMHYGTZRJYBS-UHFFFAOYSA-N
Formula: C8H14
SMILES: C1CCC2CC2CC1
Mol. weight [g/mol]: 110.20
CAS: 286-43-1

Physical Properties

Property code	Value	Unit	Source
chl	-5089.00 ± 1.00	kJ/mol	NIST Webbook
gf	113.78	kJ/mol	Joback Method
hf	-17.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-60.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.55	kJ/mol	Joback Method
hvap	43.50 ± 0.80	kJ/mol	NIST Webbook
hvap	43.50 ± 0.80	kJ/mol	NIST Webbook
hvap	43.00	kJ/mol	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	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	888.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	1045.00		NIST Webbook
tb	414.00 ± 3.00	K	NIST Webbook
tc	614.38	K	Joback Method
tf	208.76	K	Joback Method
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
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

Sources

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=C286431&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume