Bicyclo[2.1.0]pentane

Inchi: InChI=1S/C5H8/c1-2-5-3-4(1)5/h4-5H,1-3H2
InchiKey: MHLPKAGDPWUOOT-UHFFFAOYSA-N
Formula: C5H8
SMILES: C1CC2CC12
Mol. weight [g/mol]: 68.12
CAS: 185-94-4

Physical Properties

Property code	Value	Unit	Source
gf	124.82	kJ/mol	Joback Method
hf	158.00	kJ/mol	NIST Webbook
hfus	7.08	kJ/mol	Joback Method
hvap	28.00 ± 0.50	kJ/mol	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.416		Crippen Method
mcvol	59.590	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	318.60	K	NIST Webbook
tc	509.85	K	Joback Method
tf	185.51	K	Joback Method
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.86	J/mol×K	323.01	Joback Method
cpg	102.94	J/mol×K	354.15	Joback Method
cpg	114.16	J/mol×K	385.29	Joback Method
cpg	124.57	J/mol×K	416.43	Joback Method
cpg	134.23	J/mol×K	447.57	Joback Method
cpg	143.19	J/mol×K	478.71	Joback Method
cpg	151.49	J/mol×K	509.85	Joback Method

dvisc	0.0000850	Pa×s	185.51	Joback Method
dvisc	0.0001119	Pa×s	208.43	Joback Method
dvisc	0.0001395	Pa×s	231.34	Joback Method
dvisc	0.0001671	Pa×s	254.26	Joback Method
dvisc	0.0001943	Pa×s	277.18	Joback Method
dvisc	0.0002208	Pa×s	300.09	Joback Method
dvisc	0.0002464	Pa×s	323.01	Joback Method
hvapt	28.60	kJ/mol	305.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C185944&Units=SI
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume