

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	m ³ /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	Paxs	185.51	Joback Method
dvisc	0.0001119	Paxs	208.43	Joback Method
dvisc	0.0001395	Paxs	231.34	Joback Method
dvisc	0.0001671	Paxs	254.26	Joback Method
dvisc	0.0001943	Paxs	277.18	Joback Method
dvisc	0.0002208	Paxs	300.09	Joback Method
dvisc	0.0002464	Paxs	323.01	Joback Method
hvapt	28.60	kJ/mol	305.50	NIST Webbook

Sources

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=C185944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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