

Bicyclo[4.3.0]nonane, isomer # 1

Inchi: InChI=1S/C9H16/c1-2-5-9-7-3-6-8(9)4-1/h8-9H,1-7H2
InchiKey: BNRNAKTVFSZAFA-UHFFFAOYSA-N
Formula: C9H16
SMILES: C1CCC2CCCC2C1
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	110.10	kJ/mol	Joback Method
hf	-101.97	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	35.97	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.977		Crippen Method
mcvol	115.950	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	963.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	975.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1086.00		NIST Webbook
tb	431.61	K	Joback Method
tc	647.88	K	Joback Method
tf	216.51	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.94	J/molxK	431.61	Joback Method
cpg	261.35	J/molxK	467.66	Joback Method
cpg	280.52	J/molxK	503.70	Joback Method
cpg	298.50	J/molxK	539.75	Joback Method
cpg	315.35	J/molxK	575.79	Joback Method

cpg	331.12	J/molxK	611.84	Joback Method
cpg	345.88	J/molxK	647.88	Joback Method
dvisc	0.0026731	Paxs	216.51	Joback Method
dvisc	0.0016168	Paxs	252.36	Joback Method
dvisc	0.0011082	Paxs	288.21	Joback Method
dvisc	0.0008258	Paxs	324.06	Joback Method
dvisc	0.0006525	Paxs	359.91	Joback Method
dvisc	0.0005380	Paxs	395.76	Joback Method
dvisc	0.0004581	Paxs	431.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R524433&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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