CIS-BICYCLO[4.3.0]-3-NONENE

Other names: 2,3,3a,4,7,7a-Hexahydro-1H-indene
Inchi: InChI=1S/C9H14/c1-2-5-9-7-3-6-8(9)4-1/h1-2,8-9H,3-7H2/t8-,9+
InchiKey: UZURTQHPMXADGG-UHFFFAOYSA-N
Formula: C9H14
SMILES: C1=CC[C@H]2CCC[C@H]2C1
Mol. weight [g/mol]: 122.21

Physical Properties

Property code	Value	Unit	Source
hf	10.30	kJ/mol	Cheméo Relay (1.0)
hfus	10.26	kJ/mol	Joback Method
hvap	50.45	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-4.38		Cheméo Relay (1.0)
logp	2.753		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1038.00		NIST Webbook
tb	430.94	K	Cheméo Relay (1.0)
tc	694.68	K	Cheméo Relay (1.0)
tf	253.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.80	J/mol×K	430.77	Joback Method
cpg	324.39	J/mol×K	649.36	Joback Method
cpg	310.78	J/mol×K	612.93	Joback Method
cpg	296.19	J/mol×K	576.50	Joback Method
cpg	280.56	J/mol×K	540.06	Joback Method
cpg	263.83	J/mol×K	503.63	Joback Method
cpg	245.93	J/mol×K	467.20	Joback Method
dvisc	0.0007327	Pa×s	324.02	Joback Method
dvisc	0.0004387	Pa×s	430.77	Joback Method

dvisc	0.0005047	Pa×s	395.19	Joback Method
dvisc	0.0005970	Pa×s	359.60	Joback Method
dvisc	0.0020254	Pa×s	217.27	Joback Method
dvisc	0.0009458	Pa×s	288.44	Joback Method
dvisc	0.0013118	Pa×s	252.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85236788&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point