

Bicyclo[4.2.1]non-3-en-9-ol, anti-

Inchi:	InChI=1S/C9H14O/c10-9-7-3-1-2-4-8(9)6-5-7/h1-2,7-10H,3-6H2
InchiKey:	KHYZIIYIOGSVEHF-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	OC1C2CC=CCC1CC2
Mol. weight [g/mol]:	138.21
CAS:	64725-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-4.47	kJ/mol	Joback Method
hf	-216.76	kJ/mol	Joback Method
hfus	15.42	kJ/mol	Joback Method
hvap	52.63	kJ/mol	Joback Method
ie	9.11 ± 0.02	eV	NIST Webbook
log10ws	-2.12		Crippen Method
logp	1.723		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	518.28	K	Joback Method
tc	722.51	K	Joback Method
tf	273.85	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.96	J/molxK	518.28	Joback Method
cpg	360.22	J/molxK	688.47	Joback Method
cpg	347.90	J/molxK	654.44	Joback Method
cpg	334.76	J/molxK	620.40	Joback Method
cpg	320.76	J/molxK	586.36	Joback Method
cpg	305.84	J/molxK	552.32	Joback Method
cpg	371.75	J/molxK	722.51	Joback Method
dvisc	0.0003225	Paxs	518.28	Joback Method

dvisc	0.0004588	Paxs	477.54	Joback Method
dvisc	0.0006972	Paxs	436.80	Joback Method
dvisc	0.0011547	Paxs	396.06	Joback Method
dvisc	0.0021470	Paxs	355.33	Joback Method
dvisc	0.0046873	Paxs	314.59	Joback Method
dvisc	0.0129096	Paxs	273.85	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=C64725582&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
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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