

Bicyclo[2.2.1]hept-5-en-2-ol, 2-ethenyl-, (exo)-

Inchi:	InChI=1S/C9H12O/c1-2-9(10)6-7-3-4-8(9)5-7/h2-4,7-8,10H,1,5-6H2/t7?,8?,9-/m1/s1
InchiKey:	YZIBFCLJXJRCHE-AMDVSUOASA-N
Formula:	C9H12O
SMILES:	C=CC1(O)CC2C=CC1C2
Mol. weight [g/mol]:	136.19
CAS:	37165-53-0

Physical Properties

Property code	Value	Unit	Source
gf	102.08	kJ/mol	Joback Method
hf	-63.77	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	50.47	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.499		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	506.66	K	Joback Method
tc	708.70	K	Joback Method
tf	303.03	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.44	J/mol×K	506.66	Joback Method
cpg	284.82	J/mol×K	540.33	Joback Method
cpg	297.16	J/mol×K	574.01	Joback Method
cpg	308.59	J/mol×K	607.68	Joback Method
cpg	319.22	J/mol×K	641.35	Joback Method
cpg	329.21	J/mol×K	675.02	Joback Method
cpg	338.66	J/mol×K	708.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C37165530&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
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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