

Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 «alpha»,4 «alpha»,5 «alpha»)-

Inchi:	InChI=1S/C10H14/c1-2-9-7-8-3-5-10(9)6-4-8/h2-3,5,8-10H,1,4,6-7H2/t8-,9-,10-/m0/s1
InchiKey:	OVAIKAHQOHGBD-GUBZILKMSA-N
Formula:	C10H14
SMILES:	C=CC1CC2C=CC1CC2
Mol. weight [g/mol]:	134.22
CAS:	21145-79-9

Physical Properties

Property code	Value	Unit	Source
gf	240.71	kJ/mol	Joback Method
hf	105.00 ± 4.20	kJ/mol	NIST Webbook
hf	106.00	kJ/mol	NIST Webbook
hfus	14.74	kJ/mol	Joback Method
hvap	37.34	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.775		Crippen Method
mcvol	121.440	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	441.39	K	Joback Method
tc	652.99	K	Joback Method
tf	226.06	K	Joback Method
vc	0.460	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.67	J/molxK	441.39	Joback Method
cpg	336.92	J/molxK	617.72	Joback Method
cpg	322.61	J/molxK	582.45	Joback Method
cpg	307.28	J/molxK	547.19	Joback Method
cpg	290.90	J/molxK	511.92	Joback Method
cpg	273.38	J/molxK	476.66	Joback Method
cpg	350.30	J/molxK	652.99	Joback Method
dvisc	0.0005064	Paxs	441.39	Joback Method

dvisc	0.0005312	Paxs	405.50	Joback Method
dvisc	0.0005624	Paxs	369.61	Joback Method
dvisc	0.0006028	Paxs	333.73	Joback Method
dvisc	0.0006570	Paxs	297.84	Joback Method
dvisc	0.0007332	Paxs	261.95	Joback Method
dvisc	0.0008472	Paxs	226.06	Joback Method

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=C21145799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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