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

Inchi: InChI=1S/C9H14/c1-7-6-8-2-4-9(7)5-3-8/h2,4,7-9H,3,5-6H2,1H3/t7-,8?,9?/m1/s1
InchiKey: XOGBWGJGWDPLQZ-AFPNSQJFSA-N
Formula: C9H14
SMILES: CC1CC2C=CC1CC2
Mol. weight [g/mol]: 122.21
CAS: 14803-42-0

Physical Properties

Property code	Value	Unit	Source
gf	144.45	kJ/mol	Joback Method
hf	-1.00 ± 4.20	kJ/mol	NIST Webbook
hfus	13.43	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.609		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	421.83	K	Joback Method
tc	631.22	K	Joback Method
tf	216.55	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.58	J/mol×K	421.83	Joback Method
cpg	245.95	J/mol×K	456.73	Joback Method
cpg	263.20	J/mol×K	491.63	Joback Method
cpg	279.39	J/mol×K	526.53	Joback Method
cpg	294.58	J/mol×K	561.43	Joback Method
cpg	308.82	J/mol×K	596.32	Joback Method
cpg	322.16	J/mol×K	631.22	Joback Method
dvisc	0.0007519	Pa×s	216.55	Joback Method
dvisc	0.0006590	Pa×s	250.76	Joback Method

dvisc	0.0005961	Pa×s	284.98	Joback Method
dvisc	0.0005509	Pa×s	319.19	Joback Method
dvisc	0.0005170	Pa×s	353.40	Joback Method
dvisc	0.0004906	Pa×s	387.62	Joback Method
dvisc	0.0004696	Pa×s	421.83	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=C14803420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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