Bicyclo[2.2.2]oct-5-en-2-ol-(1«alpha»,2«beta»,4«a

Inchi: InChI=1S/C8H12O/c9-8-5-6-1-3-7(8)4-2-6/h1,3,6-9H,2,4-5H2/t6?,7?,8-/m1/s1
InchiKey: KEXYAVHJBNJUCG-KAVNDROISA-N
Formula: C8H12O
SMILES: OC1CC2C=CC1CC2
Mol. weight [g/mol]: 124.18
CAS: 19245-72-8

Physical Properties

Property code	Value	Unit	Source
gf	-0.79	kJ/mol	Joback Method
hf	-189.96	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Joback Method
ie	9.25 ± 0.02	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.333		Crippen Method
mcvol	103.430	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	491.13	K	Joback Method
tc	690.84	K	Joback Method
tf	266.10	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.73	J/mol×K	491.13	Joback Method
cpg	258.94	J/mol×K	524.41	Joback Method
cpg	272.27	J/mol×K	557.70	Joback Method
cpg	284.78	J/mol×K	590.98	Joback Method
cpg	296.52	J/mol×K	624.27	Joback Method
cpg	307.51	J/mol×K	657.55	Joback Method
cpg	317.83	J/mol×K	690.84	Joback Method
dvisc	0.0101870	Pa×s	266.10	Joback Method

dvisc	0.0043461	Pa×s	303.61	Joback Method
dvisc	0.0022362	Pa×s	341.11	Joback Method
dvisc	0.0013125	Pa×s	378.62	Joback Method
dvisc	0.0008480	Pa×s	416.12	Joback Method
dvisc	0.0005889	Pa×s	453.62	Joback Method
dvisc	0.0004324	Pa×s	491.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C19245728&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