

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

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-/m0/s1
InchiKey:	KEXYAVHJBNJUCG-RRQHEKLDSA-N
Formula:	C8H12O
SMILES:	OC1CC2C=CC1CC2
Mol. weight [g/mol]:	124.18
CAS:	6688-07-9

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	9.14 ± 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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0043461	Paxs	303.61	Joback Method
dvisc	0.0022362	Paxs	341.11	Joback Method
dvisc	0.0013125	Paxs	378.62	Joback Method
dvisc	0.0008480	Paxs	416.12	Joback Method
dvisc	0.0005889	Paxs	453.62	Joback Method
dvisc	0.0004324	Paxs	491.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6688079&Units=SI
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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