cis-Bicyclo[3.3.0]oct-2-ene

Other names:	cis-Bicyclo[3.3.0]-2-octene
	Pentalene, 1,2,3,3a,4,6a-hexahydro-, cis-
	1,2,3,3a,4,6a-Hexahydropentalene, (Z)-
	cis-1,2,3,3a,4,6a-hexahydropentalene
Inchi:	InChI=1S/C8H12/c1-3-7-5-2-6-8(7)4-1/h1,3,7-8H,2,4-6H2/t7-,8+/m1/s1
InchiKey:	KEHFJHPSOFFXBO-SFYZADRCSA-N
Formula:	C8H12
SMILES:	C1=CC2CCCC2C1
Mol. weight [g/mol]:	108.18
CAS:	930-99-4

Physical Properties

Property code	Value	Unit	Source
gf	143.74	kJ/mol	Joback Method
hf	-17.39	kJ/mol	Joback Method
hfus	9.77	kJ/mol	Joback Method
hvap	33.86	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.363		Crippen Method
mcvol	97.560	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	853.90		NIST Webbook
rinpol	848.70		NIST Webbook
rinpol	875.10		NIST Webbook
rinpol	867.80		NIST Webbook
tb	403.62	K	Joback Method
tc	615.80	K	Joback Method
tf	209.52	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.77	J/mol×K	403.62	Joback Method
cpg	202.83	J/mol×K	438.98	Joback Method
cpg	218.77	J/mol×K	474.35	Joback Method
cpg	233.66	J/mol×K	509.71	Joback Method
cpg	247.55	J/mol×K	545.07	Joback Method
cpg	260.50	J/mol×K	580.43	Joback Method
cpg	272.57	J/mol×K	615.80	Joback Method
dvisc	0.0010286	Pa×s	209.52	Joback Method
dvisc	0.0008159	Pa×s	241.87	Joback Method
dvisc	0.0006835	Pa×s	274.22	Joback Method
dvisc	0.0005944	Pa×s	306.57	Joback Method
dvisc	0.0005308	Pa×s	338.92	Joback Method
dvisc	0.0004835	Pa×s	371.27	Joback Method
dvisc	0.0004471	Pa×s	403.62	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C930994&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume