

Bicyclo(3.2.1)oct-2-ene

Other names:	Bicyclo(3.2.1)-2-octene
Inchi:	InChI=1S/C8H12/c1-2-7-4-5-8(3-1)6-7/h1-2,7-8H,3-6H2
InchiKey:	YEHSTKKZWWSIMD-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C1=CC2CCC(C1)C2
Mol. weight [g/mol]:	108.18
CAS:	823-02-9

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
ie	8.76 ± 0.02	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.363		Crippen Method
mcvol	97.560	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
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	260.50	J/mol×K	580.43	Joback Method
cpg	247.55	J/mol×K	545.07	Joback Method
cpg	233.66	J/mol×K	509.71	Joback Method
cpg	218.77	J/mol×K	474.35	Joback Method
cpg	202.83	J/mol×K	438.98	Joback Method
cpg	272.57	J/mol×K	615.80	Joback Method

dvisc	0.0004471	Pa×s	403.62	Joback Method
dvisc	0.0004835	Pa×s	371.27	Joback Method
dvisc	0.0005308	Pa×s	338.92	Joback Method
dvisc	0.0005944	Pa×s	306.57	Joback Method
dvisc	0.0006835	Pa×s	274.22	Joback Method
dvisc	0.0008159	Pa×s	241.87	Joback Method
dvisc	0.0010286	Pa×s	209.52	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	https://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C823029&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
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

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