

Bicyclo[2.2.2]octa-2,5-diene

Inchi:	InChI=1S/C8H10/c1-2-8-5-3-7(1)4-6-8/h1-3,5,7-8H,4,6H2
InchiKey:	PPABCIZFQNHUIH-UHFFFAOYSA-N
Formula:	C8H10
SMILES:	C1=CC2C=CC1CC2
Mol. weight [g/mol]:	106.17
CAS:	500-23-2

Physical Properties

Property code	Value	Unit	Source
gf	173.70	kJ/mol	Joback Method
hf	40.39	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	34.16	kJ/mol	Joback Method
ie	8.87	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.139		Crippen Method
mcvol	93.260	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	817.00		NIST Webbook
rinpol	817.00		NIST Webbook
tb	402.78	K	Joback Method
tc	617.25	K	Joback Method
tf	210.28	K	Joback Method
vc	0.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.91	J/mol×K	402.78	Joback Method
cpg	188.64	J/mol×K	438.53	Joback Method
cpg	203.27	J/mol×K	474.27	Joback Method
cpg	216.87	J/mol×K	510.02	Joback Method
cpg	229.50	J/mol×K	545.76	Joback Method
cpg	241.22	J/mol×K	581.51	Joback Method

cpg	252.10	J/mol×K	617.25	Joback Method
dvisc	0.0007709	Paxs	210.28	Joback Method
dvisc	0.0006515	Paxs	242.36	Joback Method
dvisc	0.0005727	Paxs	274.45	Joback Method
dvisc	0.0005172	Paxs	306.53	Joback Method
dvisc	0.0004762	Paxs	338.61	Joback Method
dvisc	0.0004447	Paxs	370.70	Joback Method
dvisc	0.0004199	Paxs	402.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C500232&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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