

9-Oxabicyclo[4.2.1]nona-2,4-diene

Inchi:	InChI=1S/C8H10O/c1-2-4-8-6-5-7(3-1)9-8/h1-4,7-8H,5-6H2
InchiKey:	UPTPBLCFJRDBQW-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	C1=CC2CCC(C=C1)O2
Mol. weight [g/mol]:	122.16
CAS:	19740-75-1

Physical Properties

Property code	Value	Unit	Source
gf	75.48	kJ/mol	Joback Method
hf	-97.77	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	38.84	kJ/mol	Joback Method
ie	8.55	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.660		Crippen Method
mcvol	99.130	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	434.00	K	Joback Method
tc	657.19	K	Joback Method
tf	233.33	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.64	J/molxK	434.00	Joback Method
cpg	217.67	J/molxK	471.20	Joback Method
cpg	232.58	J/molxK	508.40	Joback Method
cpg	246.45	J/molxK	545.60	Joback Method
cpg	259.32	J/molxK	582.79	Joback Method
cpg	271.26	J/molxK	619.99	Joback Method
cpg	282.34	J/molxK	657.19	Joback Method
dvisc	0.0019904	Paxs	233.33	Joback Method

dvisc	0.0013610	Paxs	266.78	Joback Method
dvisc	0.0010128	Paxs	300.22	Joback Method
dvisc	0.0007997	Paxs	333.67	Joback Method
dvisc	0.0006593	Paxs	367.11	Joback Method
dvisc	0.0005613	Paxs	400.56	Joback Method
dvisc	0.0004898	Paxs	434.00	Joback Method

Sources

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=C19740751&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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