

Bicyclo[4.2.1]nona-2,4-dien-9-ol, anti-

Inchi:	InChI=1S/C9H12O/c10-9-7-3-1-2-4-8(9)6-5-7/h1-4,7-10H,5-6H2
InchiKey:	LSLWFYJHUWVPVQR-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	OC1C2C=CC=CC1CC2
Mol. weight [g/mol]:	136.19
CAS:	64725-60-6

Physical Properties

Property code	Value	Unit	Source
gf	25.49	kJ/mol	Joback Method
hf	-158.98	kJ/mol	Joback Method
hfus	16.64	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
ie	8.43 ± 0.02	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.499		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	517.44	K	Joback Method
tc	723.65	K	Joback Method
tf	274.61	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.35	J/mol×K	517.44	Joback Method
cpg	287.07	J/mol×K	551.81	Joback Method
cpg	300.85	J/mol×K	586.18	Joback Method
cpg	313.75	J/mol×K	620.54	Joback Method
cpg	325.82	J/mol×K	654.91	Joback Method
cpg	337.10	J/mol×K	689.28	Joback Method
cpg	347.63	J/mol×K	723.65	Joback Method
dvisc	0.0106431	Pa×s	274.61	Joback Method

dvisc	0.0040861	Pa×s	315.08	Joback Method
dvisc	0.0019507	Pa×s	355.55	Joback Method
dvisc	0.0010832	Pa×s	396.03	Joback Method
dvisc	0.0006708	Pa×s	436.50	Joback Method
dvisc	0.0004506	Pa×s	476.97	Joback Method
dvisc	0.0003221	Pa×s	517.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64725606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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