

Tricyclo[4.2.1.0^{2,5}]nona-3,7-diene,(1 «alpha»,2 «beta»)

Inchi:	InChI=1S/C9H10/c1-2-7-5-6(1)8-3-4-9(7)8/h1-4,6-9H,5H2/t6-,7+,8+,9-
InchiKey:	KXHIYQZTTRKYGP-OJOKCITNSA-N
Formula:	C9H10
SMILES:	C1=CC2CC1C1C=CC21
Mol. weight [g/mol]:	118.18
CAS:	15564-44-0

Physical Properties

Property code	Value	Unit	Source
gf	259.36	kJ/mol	Joback Method
hf	84.53	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	35.64	kJ/mol	Joback Method
ie	8.65 ± 0.05	eV	NIST Webbook
log10ws	-2.01		Crippen Method
logp	1.994		Crippen Method
mcvol	96.490	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	419.19	K	Joback Method
tc	631.31	K	Joback Method
tf	242.29	K	Joback Method
vc	0.382	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.01	J/molxK	419.19	Joback Method
cpg	272.35	J/molxK	595.95	Joback Method
cpg	260.37	J/molxK	560.60	Joback Method
cpg	247.34	J/molxK	525.25	Joback Method
cpg	233.17	J/molxK	489.90	Joback Method
cpg	217.76	J/molxK	454.54	Joback Method
cpg	283.40	J/molxK	631.31	Joback Method
dvisc	0.0009037	Paxs	419.19	Joback Method

dvisc	0.0007781	Paxs	389.71	Joback Method
dvisc	0.0006538	Paxs	360.22	Joback Method
dvisc	0.0005325	Paxs	330.74	Joback Method
dvisc	0.0004167	Paxs	301.26	Joback Method
dvisc	0.0003092	Paxs	271.77	Joback Method
dvisc	0.0002133	Paxs	242.29	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=C15564440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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<https://www.chemeo.com/cid/33-346-1/Tricyclo-4-2-1-02-5-nona-3-7-diene-1-alpha-2-beta-5-beta-6-alpha.pdf>

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