

1,8-Nonadiene

Other names:	nona-1,8-diene
Inchi:	InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h3-4H,1-2,5-9H2
InchiKey:	VJHGSLHHMIELQD-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	C=CCCCCCC=C
Mol. weight [g/mol]:	124.22
CAS:	4900-30-5

Physical Properties

Property code	Value	Unit	Source
gf	200.58	kJ/mol	Joback Method
hf	21.77	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	34.29	kJ/mol	Joback Method
ie	9.51 ± 0.02	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	862.70		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	882.00		NIST Webbook
tb	416.00 ± 4.00	K	NIST Webbook
tb	413.00 ± 2.00	K	NIST Webbook
tb	415.00 ± 2.00	K	NIST Webbook
tb	415.70	K	NIST Webbook
tc	568.34	K	Joback Method
tf	187.67	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.13	J/mol×K	398.68	Joback Method
cpg	255.23	J/mol×K	426.96	Joback Method
cpg	267.78	J/mol×K	455.23	Joback Method
cpg	279.79	J/mol×K	483.51	Joback Method
cpg	291.30	J/mol×K	511.79	Joback Method
cpg	302.30	J/mol×K	540.07	Joback Method
cpg	312.82	J/mol×K	568.34	Joback Method
dvisc	0.0042470	Paxs	187.67	Joback Method
dvisc	0.0017898	Paxs	222.84	Joback Method
dvisc	0.0009546	Paxs	258.01	Joback Method
dvisc	0.0005920	Paxs	293.18	Joback Method
dvisc	0.0004067	Paxs	328.34	Joback Method
dvisc	0.0003005	Paxs	363.51	Joback Method
dvisc	0.0002342	Paxs	398.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55780e+01
Coeff. B	-3.93452e+03
Coeff. C	-5.67010e+01
Temperature range (K), min.	314.02
Temperature range (K), max.	439.94

Sources

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=C4900305&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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