

1,3-Nonadiene, (E)-

Other names:	(E)-n-C ₅ H ₁₁ CH=CHCH=CH ₂ (E)-1,3-Nonadiene (3E)-1,3-Nonadiene 1,trans-3-Nonadiene trans-1,3-Nonadiene
Inchi:	InChI=1S/C ₉ H ₁₆ /c1-3-5-7-9-8-6-4-2/h3,5,7H,1,4,6,8-9H ₂ ,2H ₃ /b7-5+
InchiKey:	CLNYHERYALISIR-FNORWQNLSA-N
Formula:	C ₉ H ₁₆
SMILES:	C=CC=CCCCCC
Mol. weight [g/mol]:	124.22
CAS:	56700-77-7

Physical Properties

Property code	Value	Unit	Source
gf	192.96	kJ/mol	Joback Method
hf	13.56	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	34.92	kJ/mol	Joback Method
ie	8.44	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	909.70		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	909.70		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1045.00		NIST Webbook
tb	406.16	K	Joback Method
tc	580.81	K	Joback Method
tf	184.35	K	Joback Method
vc	0.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.68	J/molxK	406.16	Joback Method
cpg	304.08	J/molxK	551.71	Joback Method
cpg	292.93	J/molxK	522.60	Joback Method
cpg	281.24	J/molxK	493.49	Joback Method
cpg	268.99	J/molxK	464.38	Joback Method
cpg	256.14	J/molxK	435.27	Joback Method
cpg	314.71	J/molxK	580.81	Joback Method
dvisc	0.0001978	Paxs	406.16	Joback Method
dvisc	0.0002575	Paxs	369.19	Joback Method
dvisc	0.0003554	Paxs	332.22	Joback Method
dvisc	0.0005317	Paxs	295.25	Joback Method
dvisc	0.0008927	Paxs	258.29	Joback Method
dvisc	0.0017822	Paxs	221.32	Joback Method
dvisc	0.0046945	Paxs	184.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56700777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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