

2-Nonenal, (E)-

Other names:	(2E)-2-Nonenal (2E)nonenal (E)-2-Nonen-1-al (E)-2-Nonenal (E)-Non-2-enal 2E-Nonen-1-al Non-2-(E)-enal t-2-Nonenal trans-2-Nonen-1-al trans-2-Nonenal trans-Non-2-enal
Inchi:	InChI=1S/C9H16O/c1-2-3-4-5-6-7-8-9-10/h7-9H,2-6H2,1H3/b8-7+
InchiKey:	BSAIUMLZVGUGKX-BQYQJAHWSA-N
Formula:	C9H16O
SMILES:	CCCCCCC=CC=O
Mol. weight [g/mol]:	140.22
CAS:	18829-56-6

Physical Properties

Property code	Value	Unit	Source
gf	5.60	kJ/mol	Joback Method
hf	-197.45	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
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tf	228.11	K	Joback Method
vc	0.536	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.41	J/molxK	635.79	Joback Method
cpg	341.26	J/molxK	606.18	Joback Method
cpg	330.61	J/molxK	576.57	Joback Method
cpg	319.44	J/molxK	546.97	Joback Method
cpg	307.72	J/molxK	517.36	Joback Method
cpg	295.43	J/molxK	487.75	Joback Method
cpg	282.56	J/molxK	458.14	Joback Method
dvisc	0.0047317	Paxs	228.11	Joback Method
dvisc	0.0002551	Paxs	458.14	Joback Method
dvisc	0.0003323	Paxs	419.80	Joback Method
dvisc	0.0004566	Paxs	381.46	Joback Method
dvisc	0.0006735	Paxs	343.12	Joback Method
dvisc	0.0010953	Paxs	304.79	Joback Method
dvisc	0.0020491	Paxs	266.45	Joback Method
hvapt	56.10	kJ/mol	380.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47150e+01
Coeff. B	-4.10316e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	357.92
Temperature range (K), max.	509.86

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=C18829566&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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