

3-nonynoic acid

Inchi:	InChI=1S/C9H14O2/c1-2-3-4-5-6-7-8-9(10)11/h2-5,8H2,1H3,(H,10,11)
InchiKey:	ZGMVHFLYJANFQJ-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CCCCC#CCC(=O)O
Mol. weight [g/mol]:	154.21
CAS:	56630-33-2

Physical Properties

Property code	Value	Unit	Source
gf	-38.04	kJ/mol	Joback Method
hf	-301.76	kJ/mol	Cheméo Relay (1.0)
hfus	27.88	kJ/mol	Joback Method
hvap	83.60	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-1.86		Cheméo Relay (1.0)
logp	2.045		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	521.35	K	Cheméo Relay (1.0)
tc	709.54	K	Cheméo Relay (1.0)
tf	295.85	K	Cheméo Relay (1.0)
vc	0.477	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.89	J/mol×K	560.37	Joback Method
cpg	328.66	J/mol×K	591.44	Joback Method
cpg	338.94	J/mol×K	622.52	Joback Method
cpg	348.75	J/mol×K	653.59	Joback Method
cpg	358.10	J/mol×K	684.67	Joback Method
cpg	367.00	J/mol×K	715.74	Joback Method
cpg	375.48	J/mol×K	746.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57239e+01
Coeff. B	-5.31769e+03
Coeff. C	-1.02860e+02
Temperature range (K), min.	447.15
Temperature range (K), max.	613.15

Sources

The Yaws Handbook of Vapor Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
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
pvap: Vapor pressure

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

Latest version available from:

<https://www.cheméo.com/cid/105-673-8/3-nonynoic-acid.pdf>

Generated by Cheméo on 2026-07-22 00:13:18.655091117 +0000 UTC m=+190294.496976513.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.