1-Nonen-4-yne

Inchi: InChI=1S/C9H14/c1-3-5-7-9-8-6-4-2/h3H,1,4-6,8H2,2H3
InchiKey: GCZWNQLPRSOVNI-UHFFFAOYSA-N
Formula: C9H14
SMILES: C=CCC#CCCCC
Mol. weight [g/mol]: 122.21
CAS: 31508-12-0

Physical Properties

Property code	Value	Unit	Source
gf	315.54	kJ/mol	Joback Method
hf	168.64	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.756		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	411.00	K	Joback Method
tc	600.99	K	Joback Method
tf	295.53	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.88	J/mol×K	411.00	Joback Method
cpg	244.58	J/mol×K	442.66	Joback Method
cpg	256.72	J/mol×K	474.33	Joback Method
cpg	268.34	J/mol×K	505.99	Joback Method
cpg	279.44	J/mol×K	537.66	Joback Method
cpg	290.04	J/mol×K	569.32	Joback Method
cpg	300.17	J/mol×K	600.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.00	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38216e+01
Coeff. B	-3.48193e+03
Coeff. C	-5.74750e+01
Temperature range (K), min.	314.75
Temperature range (K), max.	466.63

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31508120&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/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

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

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