

1,8-Nonadiyne

Other names:	nona-1,8-diyne
Inchi:	InChI=1S/C9H12/c1-3-5-7-9-8-6-4-2/h1-2H,5-9H2
InchiKey:	DMOVPHYFYSASTC-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C#CCCCCCC#C
Mol. weight [g/mol]:	120.19
CAS:	2396-65-8

Physical Properties

Property code	Value	Unit	Source
gf	471.04	kJ/mol	Joback Method
hf	354.71	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	35.34	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.203		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	926.00		NIST Webbook
tb	435.20	K	NIST Webbook
tb	435.13 ± 0.20	K	NIST Webbook
tc	572.50	K	Joback Method
tf	252.00 ± 4.00	K	NIST Webbook
tf	245.87 ± 0.10	K	NIST Webbook
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.55	J/mol×K	385.56	Joback Method
cpg	232.01	J/mol×K	416.72	Joback Method
cpg	242.91	J/mol×K	447.87	Joback Method
cpg	253.26	J/mol×K	479.03	Joback Method
cpg	263.10	J/mol×K	510.19	Joback Method

cpg	272.44	J/mol×K	541.34	Joback Method
cpg	281.31	J/mol×K	572.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	328.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62720e+01
Coeff. B	-4.34773e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	334.12
Temperature range (K), max.	458.79

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396658&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

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
rinpola:	Non-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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