

3-Nonyn-1-ol

Other names:	Non-3-yn-1-ol
Inchi:	InChI=1S/C9H16O/c1-2-3-4-5-6-7-8-9-10/h10H,2-5,8-9H2,1H3
InchiKey:	TZZVRLFUTNYDEG-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CCCCC#CCCO
Mol. weight [g/mol]:	140.22
CAS:	31333-13-8

Physical Properties

Property code	Value	Unit	Source
gf	90.88	kJ/mol	Joback Method
hf	-109.02	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	54.46	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.953		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	506.50	K	Joback Method
tc	684.34	K	Joback Method
tf	358.11	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.24	J/mol×K	506.50	Joback Method
cpg	312.82	J/mol×K	536.14	Joback Method
cpg	323.94	J/mol×K	565.78	Joback Method
cpg	334.59	J/mol×K	595.42	Joback Method
cpg	344.80	J/mol×K	625.06	Joback Method
cpg	354.58	J/mol×K	654.70	Joback Method
cpg	363.94	J/mol×K	684.34	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	2.70	NIST Webbook
tbrp	384.50 ± 0.50	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63785e+01
Coeff. B	-4.93670e+03
Coeff. C	-8.01240e+01
Temperature range (K), min.	387.15
Temperature range (K), max.	526.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31333138&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

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