3-Nonyne

Other names: 3-C9H16
Inchi: InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h3-5,7,9H2,1-2H3
InchiKey: SRRDSRCWRHKEKU-UHFFFAOYSA-N
Formula: C9H16
SMILES: CCC#CCCCCC
Mol. weight [g/mol]: 124.22
CAS: 20184-89-8

Physical Properties

Property code	Value	Unit	Source
gf	227.70	kJ/mol	Joback Method
hf	42.00 ± 2.50	kJ/mol	NIST Webbook
hfus	22.19	kJ/mol	Joback Method
hvap	37.78	kJ/mol	Joback Method
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.20 ± 0.02	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	2.980		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	916.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1122.50		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1110.00		NIST Webbook
tb	429.00 ± 2.00	K	NIST Webbook
tb	431.65 ± 2.00	K	NIST Webbook
tb	429.00	K	NIST Webbook

tb	429.82 ± 0.60	K	NIST Webbook
tb	425.65 ± 2.00	K	NIST Webbook
tc	600.28	K	Joback Method
tf	297.29	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.22	J/mol×K	414.32	Joback Method
cpg	260.52	J/mol×K	445.31	Joback Method
cpg	273.31	J/mol×K	476.31	Joback Method
cpg	285.57	J/mol×K	507.30	Joback Method
cpg	297.34	J/mol×K	538.29	Joback Method
cpg	308.63	J/mol×K	569.29	Joback Method
cpg	319.44	J/mol×K	600.28	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53764e+01
Coeff. B	-3.97500e+03
Coeff. C	-6.07590e+01
Temperature range (K), min.	324.20
Temperature range (K), max.	455.70

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-3.09602e+01
Coeff. B	-2.65448e+03
Coeff. C	6.98495e+00
Coeff. D	-3.21438e-06
Temperature range (K), min.	365.15
Temperature range (K), max.	429.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol434.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20184898&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=434
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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