

1-Undecyne

Other names:	1-C ₁₁ H ₂₀ undec-1-yne
Inchi:	InChI=1S/C ₁₁ H ₂₀ /c1-3-5-7-9-11-10-8-6-4-2/h1H,4-11H ₂ ,2H ₃
InchiKey:	YVSFLVNWJIEJRV-UHFFFAOYSA-N
Formula:	C ₁₁ H ₂₀
SMILES:	C#CCCCCCCCC
Mol. weight [g/mol]:	152.28
CAS:	2243-98-3

Physical Properties

Property code	Value	Unit	Source
gf	264.81	kJ/mol	Joback Method
hf	21.53	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
ie	9.90 ± 0.02	eV	NIST Webbook
log10ws	-4.22		Crippen Method
logp	3.760		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
ripol	1096.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1116.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1329.70		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1333.00		NIST Webbook

ripol	1332.00			NIST Webbook
ripol	1332.00			NIST Webbook
ripol	1331.00			NIST Webbook
ripol	1307.80			NIST Webbook
ripol	1310.00			NIST Webbook
ripol	1329.10			NIST Webbook
ripol	1311.60			NIST Webbook
ripol	1329.70			NIST Webbook
ripol	1334.00			NIST Webbook
ripol	1331.00			NIST Webbook
ripol	1334.00			NIST Webbook
tb	469.00		K	NIST Webbook
tb	472.15 ± 3.00		K	NIST Webbook
tb	485.65 ± 4.00		K	NIST Webbook
tb	473.00 ± 8.00		K	NIST Webbook
tb	469.20		K	NIST Webbook
tc	613.50		K	Joback Method
tf	260.70		K	Joback Method
vc	0.614		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.78	J/mol×K	441.20	Joback Method
cpg	343.74	J/mol×K	469.92	Joback Method
cpg	358.09	J/mol×K	498.63	Joback Method
cpg	371.83	J/mol×K	527.35	Joback Method
cpg	385.00	J/mol×K	556.07	Joback Method
cpg	397.60	J/mol×K	584.79	Joback Method
cpg	409.66	J/mol×K	613.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44981e+01
Coeff. B	-3.98178e+03
Coeff. C	-6.51370e+01
Temperature range (K), min.	345.34
Temperature range (K), max.	498.57

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2243983&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	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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