

2-Undecyne

Other names:	2-C ₁₁ H ₂₀
Inchi:	InChI=1S/C ₁₁ H ₂₀ /c1-3-5-7-9-11-10-8-6-4-2/h3,5,7-11H ₂ ,1-2H ₃
InchiKey:	XZSXEDPHMIFYOS-UHFFFAOYSA-N
Formula:	C ₁₁ H ₂₀
SMILES:	CC#CCCCCCCCC
Mol. weight [g/mol]:	152.28
CAS:	60212-29-5

Physical Properties

Property code	Value	Unit	Source
gf	244.54	kJ/mol	Joback Method
hf	1.93	kJ/mol	Joback Method
hfus	27.37	kJ/mol	Joback Method
hvap	42.23	kJ/mol	Joback Method
ie	9.28 ± 0.02	eV	NIST Webbook
log10ws	-4.22		Crippen Method
logp	3.760		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
ripol	1140.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1355.90		NIST Webbook
ripol	1355.90		NIST Webbook
ripol	1337.40		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1330.40		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1363.00		NIST Webbook

ripol	1334.10		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1366.00		NIST Webbook
tb	478.15 ± 3.00	K	NIST Webbook
tb	477.40	K	NIST Webbook
tc	642.86	K	Joback Method
tf	319.83	K	Joback Method
vc	0.614	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.56	J/mol×K	460.08	Joback Method
cpg	347.02	J/mol×K	490.54	Joback Method
cpg	361.85	J/mol×K	521.01	Joback Method
cpg	376.06	J/mol×K	551.47	Joback Method
cpg	389.69	J/mol×K	581.93	Joback Method
cpg	402.74	J/mol×K	612.39	Joback Method
cpg	415.23	J/mol×K	642.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.40	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48265e+01
Coeff. B	-4.09832e+03
Coeff. C	-6.64640e+01
Temperature range (K), min.	348.35
Temperature range (K), max.	497.19

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=C60212295&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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