

Undecane, 4-methyl-

Other names:	4-Methylundecane
Inchi:	InChI=1S/C12H26/c1-4-6-7-8-9-11-12(3)10-5-2/h12H,4-11H2,1-3H3
InchiKey:	KNMXZGDUJVOTOC-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCCCCCCC(C)CCC
Mol. weight [g/mol]:	170.33
CAS:	2980-69-0

Physical Properties

Property code	Value	Unit	Source
gf	47.72	kJ/mol	Joback Method
hf	-296.29	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1162.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1158.60		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1160.82		NIST Webbook
rinpol	1161.04		NIST Webbook
rinpol	1161.03		NIST Webbook
rinpol	1160.03		NIST Webbook
rinpol	1160.34		NIST Webbook
rinpol	1160.35		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1162.00		NIST Webbook

rinpol	1161.20		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1160.34		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1159.00		NIST Webbook
ripol	1147.00		NIST Webbook
tb	483.00 ± 3.00	K	NIST Webbook
tc	637.74	K	Joback Method
tf	206.50 ± 2.00	K	NIST Webbook
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.90	J/molxK	473.52	Joback Method
cpg	424.06	J/molxK	500.89	Joback Method
cpg	440.58	J/molxK	528.26	Joback Method
cpg	456.45	J/molxK	555.63	Joback Method
cpg	471.71	J/molxK	583.00	Joback Method
cpg	486.36	J/molxK	610.37	Joback Method
cpg	500.43	J/molxK	637.74	Joback Method
dvisc	0.0101808	Paxs	210.00	Joback Method
dvisc	0.0030132	Paxs	253.92	Joback Method
dvisc	0.0012770	Paxs	297.84	Joback Method
dvisc	0.0006749	Paxs	341.76	Joback Method
dvisc	0.0004124	Paxs	385.68	Joback Method
dvisc	0.0002787	Paxs	429.60	Joback Method
dvisc	0.0002026	Paxs	473.52	Joback Method
hvapt	51.60	kJ/mol	420.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42064e+01
Coeff. B	-3.74738e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	360.54
Temperature range (K), max.	512.61

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=C2980690&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
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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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