Undecane, 3-methyl-

Other names:	(dl) 3-methylundecane
	2-Ethyl-decane
	3-Methylundecane
Inchi:	InChI=1S/C12H26/c1-4-6-7-8-9-10-11-12(3)5-2/h12H,4-11H2,1-3H3
InchiKey:	HTZWVZNRDDOFEI-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCCCCCCCC(C)CC
Mol. weight [g/mol]:	170.33
CAS:	1002-43-3

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	1165.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1169.60		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1170.00		NIST Webbook

rinpol	1173.00		NIST Webbook
rinpol	1172.20		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1172.00		NIST Webbook
tb	473.52	K	Joback Method
tc	637.74	K	Joback Method
tf	218.50 ± 2.00	K	NIST Webbook
tf	215.20 ± 5.00	K	NIST Webbook
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.90	J/mol×K	473.52	Joback Method
cpg	424.06	J/mol×K	500.89	Joback Method
cpg	440.58	J/mol×K	528.26	Joback Method
cpg	456.45	J/mol×K	555.63	Joback Method
cpg	471.71	J/mol×K	583.00	Joback Method
cpg	486.36	J/mol×K	610.37	Joback Method
cpg	500.43	J/mol×K	637.74	Joback Method
dvisc	0.0101808	Pa×s	210.00	Joback Method
dvisc	0.0030132	Pa×s	253.92	Joback Method
dvisc	0.0012770	Pa×s	297.84	Joback Method
dvisc	0.0006749	Pa×s	341.76	Joback Method
dvisc	0.0004124	Pa×s	385.68	Joback Method
dvisc	0.0002787	Pa×s	429.60	Joback Method
dvisc	0.0002026	Pa×s	473.52	Joback Method
hvapt	48.80	kJ/mol	421.00	NIST Webbook

rhol	758.60	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	751.30	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	744.00	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	736.70	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	729.30	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	721.90	kg/m3	333.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	714.40	kg/m3	343.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	707.00	kg/m3	353.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	699.40	kg/m3	363.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	691.90	kg/m3	373.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	758.30	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	751.10	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	743.90	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	736.60	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	729.30	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41901e+01
Coeff. B	-3.75824e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	361.64
Temperature range (K), max.	514.60

Sources

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=C1002433&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
Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels:	https://www.doi.org/10.1021/je400274f

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