Undecane, 2-methyl-

Other names: 2-Methylundecane
Inchi: InChI=1S/C12H26/c1-4-5-6-7-8-9-10-11-12(2)3/h12H,4-11H2,1-3H3
InchiKey: GTJOHISYCKPIMT-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCCCCCCC(C)C
Mol. weight [g/mol]: 170.33
CAS: 7045-71-8

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	1164.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.10		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.25		NIST Webbook
rinpol	1165.41		NIST Webbook
rinpol	1165.39		NIST Webbook
rinpol	1164.40		NIST Webbook
rinpol	1164.52		NIST Webbook

rinpol	1164.69		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1165.50		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1165.41		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1155.00		NIST Webbook
tb	483.20 ± 2.00	K	NIST Webbook
tb	462.36 ± 8.00	K	NIST Webbook
tc	637.74	K	Joback Method
tf	226.29 ± 0.08	K	NIST Webbook
tf	226.34 ± 0.06	K	NIST Webbook
tf	227.60 ± 2.00	K	NIST Webbook
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.43	J/mol×K	637.74	Joback Method
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
dvisc	0.0002026	Pa×s	473.52	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
hvapt	49.50	kJ/mol	420.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67068e+01
Coeff. B	-4.78616e+03
Coeff. C	-7.57020e+01
Temperature range (K), min.	367.20
Temperature range (K), max.	495.71

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7045718&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

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