

1-Undecene, 2-methyl-

Other names:	2-Methyl-1-undecene 2-methylundec-1-ene
Inchi:	InChI=1S/C12H24/c1-4-5-6-7-8-9-10-11-12(2)3/h2,4-11H2,1,3H3
InchiKey:	SJVKHZYVCVKEGM-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	<chem>C=C(C)CCCCCCCC</chem>
Mol. weight [g/mol]:	168.32
CAS:	18516-37-5

Physical Properties

Property code	Value	Unit	Source
gf	129.45	kJ/mol	Joback Method
hf	-175.37	kJ/mol	Joback Method
hfus	24.25	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.703		Crippen Method
mcpvol	175.640	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1186.00		NIST Webbook
tb	470.52	K	Joback Method
tc	637.26	K	Joback Method
tf	209.28	K	Joback Method
vc	0.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.92	J/mol×K	470.52	Joback Method
cpg	405.48	J/mol×K	498.31	Joback Method
cpg	421.39	J/mol×K	526.10	Joback Method

cpg	436.65	J/mol×K	553.89	Joback Method
cpg	451.28	J/mol×K	581.68	Joback Method
cpg	465.32	J/mol×K	609.47	Joback Method
cpg	478.77	J/mol×K	637.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48178e+01
Coeff. B	-4.14198e+03
Coeff. C	-7.43540e+01
Temperature range (K), min.	359.41
Temperature range (K), max.	510.06

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18516375&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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