3-methyl-1-undecene

Inchi: InChI=1S/C12H24/c1-4-6-7-8-9-10-11-12(3)5-2/h5,12H,2,4,6-11H2,1,3H3
InchiKey: LGTWOHHRJHHWCO-UHFFFAOYSA-N
Formula: C12H24
SMILES: C=CC(C)CCCCCCCC
Mol. weight [g/mol]: 168.32
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	135.56	kJ/mol	Joback Method
hf	-170.86	kJ/mol	Joback Method
hfus	22.03	kJ/mol	Joback Method
hvap	41.25	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.559		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1144.00		NIST Webbook
tb	470.20	K	Joback Method
tc	637.46	K	Joback Method
tf	208.24	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.11	J/mol×K	470.20	Joback Method
cpg	466.18	J/mol×K	609.58	Joback Method
cpg	452.04	J/mol×K	581.70	Joback Method
cpg	437.28	J/mol×K	553.83	Joback Method
cpg	421.88	J/mol×K	525.95	Joback Method
cpg	405.84	J/mol×K	498.08	Joback Method
cpg	479.73	J/mol×K	637.46	Joback Method
dvisc	0.0002043	Pa×s	470.20	Joback Method

dvisc	0.0002779	Pa×s	426.54	Joback Method
dvisc	0.0004054	Pa×s	382.88	Joback Method
dvisc	0.0006519	Pa×s	339.22	Joback Method
dvisc	0.0012062	Pa×s	295.56	Joback Method
dvisc	0.0027624	Pa×s	251.90	Joback Method
dvisc	0.0089547	Pa×s	208.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58798e+01
Coeff. B	-4.55444e+03
Coeff. C	-7.60220e+01
Temperature range (K), min.	368.12
Temperature range (K), max.	506.98

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=R205984&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

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

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