1,3,5-undecatriene

Other names: Undeca-1,3,5-triene (Isomer 1)
undeca-1,3,5-triene
Inchi: InChI=1S/C11H18/c1-3-5-7-9-11-10-8-6-4-2/h3,5,7,9,11H,1,4,6,8,10H2,2H3/b7-5?,11-9+
InchiKey: JQQDKNVOSLONRS-NYCRTDSVSA-N
Formula: C11H18
SMILES: C=CC=CC=CCCCCC
Mol. weight [g/mol]: 150.26
CAS: 16356-11-9

Physical Properties

Property code	Value	Unit	Source
gf	290.02	kJ/mol	Joback Method
hf	89.50	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	39.33	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.865		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1187.00		NIST Webbook
ripol	1399.00		NIST Webbook
tb	456.08	K	Joback Method
tc	636.70	K	Joback Method
tf	201.81	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	311.85	J/mol×K	456.08	Joback Method
cpg	380.11	J/mol×K	606.60	Joback Method
cpg	367.86	J/mol×K	576.49	Joback Method
cpg	354.94	J/mol×K	546.39	Joback Method
cpg	341.33	J/mol×K	516.29	Joback Method
cpg	326.98	J/mol×K	486.18	Joback Method
cpg	391.75	J/mol×K	636.70	Joback Method
dvisc	0.0001586	Pa×s	456.08	Joback Method
dvisc	0.0002093	Pa×s	413.70	Joback Method
dvisc	0.0002941	Pa×s	371.32	Joback Method
dvisc	0.0004512	Pa×s	328.95	Joback Method
dvisc	0.0007856	Pa×s	286.57	Joback Method
dvisc	0.0016581	Pa×s	244.19	Joback Method
dvisc	0.0047896	Pa×s	201.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69014e+01
Coeff. B	-4.87774e+03
Coeff. C	-7.78840e+01
Temperature range (K), min.	371.48
Temperature range (K), max.	498.74

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=C16356119&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

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