

10-Undecenal

Other names:	1-Undecen-10-al 10-Hendecenal 10-Undecen-1-al 10-Undecenyl aldehyde 10-Undecylenealdehyde Aldehyde C-11, undecylenic C-11 Aldehyde, undecylenic Hendecenal NSC 44900 Undec-10-en-1-al Undec-10-en-al Undecylenaldehyde Undecylene aldehyde Undecylenic aldehyde n-Undecylenic aldehyde
Inchi:	InChI=1S/C11H20O/c1-2-3-4-5-6-7-8-9-10-11-12/h2,11H,1,3-10H2
InchiKey:	OFHHDSQXFXLTKC-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	C=CCCCCCCCC=O
Mol. weight [g/mol]:	168.28
CAS:	112-45-8

Physical Properties

Property code	Value	Unit	Source
gf	30.06	kJ/mol	Joback Method
hf	-230.52	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.492		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1313.00		NIST Webbook

rinpol	1277.20		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1313.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	496.42	K	Joback Method
tc	666.93	K	Joback Method
tf	253.97	K	Joback Method
vc	0.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.35	J/molxK	496.42	Joback Method
cpg	384.73	J/molxK	524.84	Joback Method
cpg	398.49	J/molxK	553.26	Joback Method
cpg	411.67	J/molxK	581.67	Joback Method
cpg	424.27	J/molxK	610.09	Joback Method
cpg	436.31	J/molxK	638.51	Joback Method
cpg	447.82	J/molxK	666.93	Joback Method
dvisc	0.0047017	Paxs	253.97	Joback Method
dvisc	0.0021200	Paxs	294.38	Joback Method
dvisc	0.0011586	Paxs	334.79	Joback Method
dvisc	0.0007212	Paxs	375.19	Joback Method
dvisc	0.0004923	Paxs	415.60	Joback Method
dvisc	0.0003595	Paxs	456.01	Joback Method
dvisc	0.0002764	Paxs	496.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48436e+01

Coeff. B	-4.39806e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	385.12
Temperature range (K), max.	544.37

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112458&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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