Undecanal, 2-methyl-

Other names:	2-Methyl-1-undecanal
	2-Methylundecanal
	Aldehyde C-12
	Aldehyde M.N.A.
	MNA
	Methyl-n-nonylacetaldehyde
	Methylnonylacetaldehyde
	Methylnonylacetic aldehyde
Inchi:	InChI=1S/C12H24O/c1-3-4-5-6-7-8-9-10-12(2)11-13/h11-12H,3-10H2,1-2H3
InchiKey:	NFAVNWJJYQAGNB-UHFFFAOYSA-N
Formula:	C12H24O
SMILES:	CCCCCCCCCC(C)C=O
Mol. weight [g/mol]:	184.32
CAS:	110-41-8

Physical Properties

Property code	Value	Unit	Source
gf	-51.80	kJ/mol	Joback Method
hf	-381.87	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.962		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1349.80		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1349.80		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1353.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1636.00		NIST Webbook
tb	444.20	K	NIST Webbook
tc	691.72	K	Joback Method

tf	252.00	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.65	J/mol×K	522.18	Joback Method
cpg	510.06	J/mol×K	663.46	Joback Method
cpg	496.62	J/mol×K	635.20	Joback Method
cpg	482.58	J/mol×K	606.95	Joback Method
cpg	467.92	J/mol×K	578.69	Joback Method
cpg	452.61	J/mol×K	550.44	Joback Method
cpg	522.91	J/mol×K	691.72	Joback Method
dvisc	0.0002384	Pa×s	522.18	Joback Method
dvisc	0.0003224	Pa×s	477.15	Joback Method
dvisc	0.0004644	Pa×s	432.12	Joback Method
dvisc	0.0007282	Pa×s	387.09	Joback Method
dvisc	0.0012853	Pa×s	342.06	Joback Method
dvisc	0.0026953	Pa×s	297.03	Joback Method
dvisc	0.0073643	Pa×s	252.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55071e+01
Coeff. B	-4.74693e+03
Coeff. C	-8.55010e+01
Temperature range (K), min.	397.40
Temperature range (K), max.	551.09

Sources

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110418&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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