Dodecanal

Other names:	1-Dodecanal
	1-Dodecyl aldehyde
	Aldehyde C-12
	Aldehyde C-12, lauric
	C-12 aldehyde, lauric
	DODECANALDEHYDE
	Dodecyl aldehyde
	Duodecylic aldehyde
	LAURALDEHYDE
	Lauric aldehyde
	Laurinaldehyde
	Lauryl aldehyde
	N-LAURALDEHYDE
	NSC 46128
	n-Dodecanal
	n-Dodecyl aldehyde
	n-Dodecylic aldehyde
Inchi:	InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h12H,2-11H2,1H3
InchiKey:	HFJRKMMYBMWEAD-UHFFFAOYSA-N
Formula:	C12H24O
SMILES:	CCCCCCCCCCCC=O
Mol. weight [g/mol]:	184.32
CAS:	112-54-9

Physical Properties

Property code	Value	Unit	Source
gf	-49.36	kJ/mol	Joback Method
hf	-376.59	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	68.30 ± 0.90	kJ/mol	NIST Webbook
hvap	70.20	kJ/mol	NIST Webbook
log10ws	-4.13		Crippen Method
logp	4.106		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1412.00		NIST Webbook

rinpol	1395.00	NIST Webbook
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ripol	1701.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1735.00		NIST Webbook
tb	504.15 ± 5.00	K	NIST Webbook
tb	511.15 ± 5.00	K	NIST Webbook
tc	689.03	K	Joback Method
tf	317.00 ± 4.00	K	NIST Webbook
tf	284.00 ± 20.00	K	NIST Webbook

tf	317.70 ± 2.00	K	NIST Webbook
tf	284.30 ± 20.00	K	NIST Webbook
tf	316.00 ± 4.00	K	NIST Webbook
tf	319.00 ± 2.00	K	NIST Webbook
tf	311.90 ± 3.00	K	NIST Webbook
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.43	J/mol×K	522.62	Joback Method
cpg	452.04	J/mol×K	550.36	Joback Method
cpg	467.02	J/mol×K	578.09	Joback Method
cpg	481.39	J/mol×K	605.83	Joback Method
cpg	495.17	J/mol×K	633.56	Joback Method
cpg	508.36	J/mol×K	661.30	Joback Method
cpg	521.00	J/mol×K	689.03	Joback Method
dvisc	0.0050355	Pa×s	267.00	Joback Method
dvisc	0.0021704	Pa×s	309.60	Joback Method
dvisc	0.0011467	Pa×s	352.21	Joback Method
dvisc	0.0006953	Pa×s	394.81	Joback Method
dvisc	0.0004647	Pa×s	437.41	Joback Method
dvisc	0.0003337	Pa×s	480.02	Joback Method
dvisc	0.0002529	Pa×s	522.62	Joback Method
hvapt	56.50	kJ/mol	440.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68735e+01
Coeff. B	-5.20653e+03
Coeff. C	-8.63080e+01
Temperature range (K), min.	400.22
Temperature range (K), max.	536.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.59818e+02
Coeff. B	-1.42801e+04
Coeff. C	-2.08974e+01
Coeff. D	1.05969e-05
Temperature range (K), min.	285.15
Temperature range (K), max.	685.00

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1243.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112549&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1243

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

hvapt: Enthalpy of vaporization at a given temperature

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume