

Tridecanal

Other names:	1-Tridecanal N-TRIDECYLALDEHYDE Tridecanaldehyde Tridecane aldehyde Tridecyl aldehyde n-Tridecanal
Inchi:	InChI=1S/C13H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h13H,2-12H2,1H3
InchiKey:	BGEHHAVMRVXCGR-UHFFFAOYSA-N
Formula:	C13H26O
SMILES:	CCCCCCCCCCCCC=O
Mol. weight [g/mol]:	198.34
CAS:	10486-19-8

Physical Properties

Property code	Value	Unit	Source
gf	-40.94	kJ/mol	Joback Method
hf	-397.23	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	73.30 ± 0.40	kJ/mol	NIST Webbook
log10ws	-4.54		Crippen Method
logp	4.496		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	277.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1486.00		NIST Webbook
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ripol	1792.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1822.00		NIST Webbook
tb	553.15 ± 5.00	K	NIST Webbook
tc	710.98	K	Joback Method
tf	288.00 ± 3.00	K	NIST Webbook
tf	287.00 ± 3.00	K	NIST Webbook
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.01	J/mol×K	545.50	Joback Method
cpg	560.88	J/mol×K	683.40	Joback Method
cpg	547.15	J/mol×K	655.82	Joback Method
cpg	532.82	J/mol×K	628.24	Joback Method
cpg	517.87	J/mol×K	600.66	Joback Method
cpg	502.27	J/mol×K	573.08	Joback Method
cpg	574.02	J/mol×K	710.98	Joback Method
dvisc	0.0002325	Pa×s	545.50	Joback Method
dvisc	0.0003080	Pa×s	500.96	Joback Method
dvisc	0.0004312	Pa×s	456.42	Joback Method
dvisc	0.0006493	Pa×s	411.88	Joback Method
dvisc	0.0010795	Pa×s	367.35	Joback Method
dvisc	0.0020651	Pa×s	322.81	Joback Method
dvisc	0.0048624	Pa×s	278.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47256e+01
Coeff. B	-4.66793e+03
Coeff. C	-9.13120e+01
Temperature range (K), min.	414.62
Temperature range (K), max.	587.15

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.45197e+02
Coeff. B	-1.91915e+04
Coeff. C	-3.33820e+01
Coeff. D	1.71089e-05
Temperature range (K), min.	288.15
Temperature range (K), max.	700.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10486198&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=1244
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/mol1244.mol

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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