12-methyltridecanal

Other names: Tridecanal, 12-methyl-
Inchi: InChI=1S/C14H28O/c1-14(2)12-10-8-6-4-3-5-7-9-11-13-15/h13-14H,3-12H2,1-2H3
InchiKey: OQWNKUAZQSLNSR-UHFFFAOYSA-N
Formula: C14H28O
SMILES: CC(C)CCCCCCCCCC=O
Mol. weight [g/mol]: 212.37
CAS: 75853-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-34.96	kJ/mol	Joback Method
hf	-423.15	kJ/mol	Joback Method
hfus	30.78	kJ/mol	Joback Method
hvap	53.09	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.742		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1863.00		NIST Webbook
tb	567.94	K	Joback Method
tc	735.40	K	Joback Method
tf	274.54	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.53	J/mol×K	567.94	Joback Method
cpg	616.41	J/mol×K	707.49	Joback Method
cpg	601.99	J/mol×K	679.58	Joback Method
cpg	586.91	J/mol×K	651.67	Joback Method
cpg	571.15	J/mol×K	623.76	Joback Method
cpg	554.70	J/mol×K	595.85	Joback Method
cpg	630.19	J/mol×K	735.40	Joback Method
dvisc	0.0001986	Pa×s	567.94	Joback Method
dvisc	0.0002704	Pa×s	519.04	Joback Method
dvisc	0.0003924	Pa×s	470.14	Joback Method
dvisc	0.0006210	Pa×s	421.24	Joback Method
dvisc	0.0011087	Pa×s	372.34	Joback Method
dvisc	0.0023587	Pa×s	323.44	Joback Method
dvisc	0.0065661	Pa×s	274.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51267e+01
Coeff. B	-4.85293e+03
Coeff. C	-9.35630e+01
Temperature range (K), min.	420.60
Temperature range (K), max.	587.99

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75853495&Units=SI

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