1-Acetoxynonadecane

Other names: Nonadecyl acetate
Inchi: InChI=1S/C21H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-21(2)22/h3
InchiKey: ZFVGKJKNNMIUDD-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 326.56
CAS: 1577-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-107.98	kJ/mol	Joback Method
hf	-721.57	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.201		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2307.70		NIST Webbook
tb	756.17	K	Joback Method
tc	929.77	K	Joback Method
tf	398.59	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.32	J/mol×K	756.17	Joback Method
cpg	1060.46	J/mol×K	900.83	Joback Method
cpg	1044.06	J/mol×K	871.90	Joback Method
cpg	1026.77	J/mol×K	842.97	Joback Method
cpg	1008.57	J/mol×K	814.04	Joback Method
cpg	989.43	J/mol×K	785.10	Joback Method
cpg	1075.99	J/mol×K	929.77	Joback Method

dvisc	0.0000640	Pa×s	756.17	Joback Method
dvisc	0.0000864	Pa×s	696.57	Joback Method
dvisc	0.0001235	Pa×s	636.98	Joback Method
dvisc	0.0001899	Pa×s	577.38	Joback Method
dvisc	0.0003224	Pa×s	517.78	Joback Method
dvisc	0.0006283	Pa×s	458.19	Joback Method
dvisc	0.0014949	Pa×s	398.59	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.79107e+01
Coeff. B	-1.15293e+04
Coeff. C	-1.42742e+02
Temperature range (K), min.	560.12
Temperature range (K), max.	652.90

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1577431&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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume