9-Decenoic acid

Other names: Caproleic acid
Dec-9-enoic acid
Inchi: InChI=1S/C10H18O2/c1-2-3-4-5-6-7-8-9-10(11)12/h2H,1,3-9H2,(H,11,12)
InchiKey: KHAVLLBUVKBTBG-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: C=CCCCCCCCC(=O)O
Mol. weight [g/mol]: 170.25
CAS: 14436-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-144.58	kJ/mol	Joback Method
hf	-389.11	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	60.61	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.988		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1389.20		NIST Webbook
rinpol	1358.00		NIST Webbook
ripol	2336.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2341.00		NIST Webbook
ripol	2356.00		NIST Webbook
ripol	2356.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2357.00		NIST Webbook
ripol	2348.00		NIST Webbook
ripol	2369.00		NIST Webbook
tb	570.93	K	Joback Method
tc	740.45	K	Joback Method

tf	311.45	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.62	J/mol×K	570.93	Joback Method
cpg	394.48	J/mol×K	599.18	Joback Method
cpg	405.82	J/mol×K	627.44	Joback Method
cpg	416.66	J/mol×K	655.69	Joback Method
cpg	427.00	J/mol×K	683.95	Joback Method
cpg	436.88	J/mol×K	712.20	Joback Method
cpg	446.29	J/mol×K	740.45	Joback Method
dvisc	0.0108543	Pa×s	311.45	Joback Method
dvisc	0.0031593	Pa×s	354.70	Joback Method
dvisc	0.0012025	Pa×s	397.94	Joback Method
dvisc	0.0005531	Pa×s	441.19	Joback Method
dvisc	0.0002923	Pa×s	484.44	Joback Method
dvisc	0.0001715	Pa×s	527.68	Joback Method
dvisc	0.0001090	Pa×s	570.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38286e+01
Coeff. B	-4.35701e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	412.52
Temperature range (K), max.	602.31

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=C14436329&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