3-Decenoic acid

Inchi: InChI=1S/C10H18O2/c1-2-3-4-5-6-7-8-9-10(11)12/h7-8H,2-6,9H2,1H3,(H,11,12)
InchiKey: CPVUNKGURQKKKX-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCCCCC=CCC(=O)O
Mol. weight [g/mol]: 170.25
CAS: 15469-77-9

Physical Properties

Property code	Value	Unit	Source
gf	-152.20	kJ/mol	Joback Method
hf	-397.32	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.988		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	578.41	K	Joback Method
tc	751.50	K	Joback Method
tf	308.13	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.20	J/mol×K	578.41	Joback Method
cpg	395.15	J/mol×K	607.26	Joback Method
cpg	406.55	J/mol×K	636.11	Joback Method
cpg	417.42	J/mol×K	664.96	Joback Method
cpg	427.78	J/mol×K	693.80	Joback Method
cpg	437.66	J/mol×K	722.65	Joback Method
cpg	447.07	J/mol×K	751.50	Joback Method
dvisc	0.0110783	Pa×s	308.13	Joback Method
dvisc	0.0029530	Pa×s	353.18	Joback Method

dvisc	0.0010616	Pa×s	398.22	Joback Method
dvisc	0.0004699	Pa×s	443.27	Joback Method
dvisc	0.0002417	Pa×s	488.32	Joback Method
dvisc	0.0001391	Pa×s	533.36	Joback Method
dvisc	0.0000873	Pa×s	578.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.70	K	1.50	NIST Webbook

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

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=C15469779&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

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