6-Heptenoic acid

Other names: hept-6-enoic acid
Inchi: InChI=1S/C7H12O2/c1-2-3-4-5-6-7(8)9/h2H,1,3-6H2,(H,8,9)
InchiKey: RWNJOXUVHRXHSD-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: C=CCCCCC(=O)O
Mol. weight [g/mol]: 128.17
CAS: 1119-60-4

Physical Properties

Property code	Value	Unit	Source
gf	-169.84	kJ/mol	Joback Method
hf	-327.19	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	53.93	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.817		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	496.20	K	NIST Webbook
tb	499.20	K	NIST Webbook
tc	675.50	K	Joback Method
tf	277.64	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.72	J/mol×K	502.29	Joback Method
cpg	257.03	J/mol×K	531.16	Joback Method
cpg	265.93	J/mol×K	560.03	Joback Method
cpg	274.42	J/mol×K	588.90	Joback Method
cpg	282.53	J/mol×K	617.76	Joback Method
cpg	290.26	J/mol×K	646.63	Joback Method
cpg	297.64	J/mol×K	675.50	Joback Method

dvisc	0.0184100	Pa×s	277.64	Joback Method
dvisc	0.0053894	Pa×s	315.08	Joback Method
dvisc	0.0020481	Pa×s	352.52	Joback Method
dvisc	0.0009373	Pa×s	389.96	Joback Method
dvisc	0.0004919	Pa×s	427.41	Joback Method
dvisc	0.0002864	Pa×s	464.85	Joback Method
dvisc	0.0001807	Pa×s	502.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47281e+01
Coeff. B	-4.35246e+03
Coeff. C	-7.99140e+01
Temperature range (K), min.	381.32
Temperature range (K), max.	542.12

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119604&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume