Heneicosanoic acid

Other names: henicosanoic acid
n-Heneicosanoic acid
Inchi: InChI=1S/C21H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23/h2
InchiKey: CKDDRHZIAZRDBW-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 326.56
CAS: 2363-71-5

Physical Properties

Property code	Value	Unit	Source
gf	-139.80	kJ/mol	Joback Method
hf	-741.58	kJ/mol	Joback Method
hfus	55.83	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.503		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	2463.20		NIST Webbook
tb	825.93	K	Joback Method
tc	1011.18	K	Joback Method
tf	347.65 ± 2.00	K	NIST Webbook
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.16	J/mol×K	980.30	Joback Method
cpg	1115.55	J/mol×K	1011.18	Joback Method
cpg	1016.16	J/mol×K	825.93	Joback Method
cpg	1035.04	J/mol×K	856.80	Joback Method
cpg	1052.93	J/mol×K	887.68	Joback Method
cpg	1069.89	J/mol×K	918.55	Joback Method

cpg	1085.95	J/mol×K	949.43	Joback Method
dvisc	0.0000141	Pa×s	825.93	Joback Method
dvisc	0.0000218	Pa×s	761.14	Joback Method
dvisc	0.0013730	Pa×s	437.18	Joback Method
dvisc	0.0003911	Pa×s	501.97	Joback Method
dvisc	0.0001484	Pa×s	566.76	Joback Method
dvisc	0.0000687	Pa×s	631.55	Joback Method
dvisc	0.0000367	Pa×s	696.35	Joback Method
hfust	63.00	kJ/mol	346.70	NIST Webbook
hvapt	149.20	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.87163e+01
Coeff. B	-7.56794e+03
Coeff. C	-1.38099e+02
Temperature range (K), min.	548.76
Temperature range (K), max.	702.67

Sources

Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c
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=C2363715&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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