17-Octadecynoic acid

Inchi: InChI=1S/C18H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h1H,3-17H2
InchiKey: DZIILFGADWDKMF-UHFFFAOYSA-N
Formula: C18H32O2
SMILES: C#CCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 280.45
CAS: 34450-18-5

Physical Properties

Property code	Value	Unit	Source
gf	58.01	kJ/mol	Joback Method
hf	-387.76	kJ/mol	Joback Method
hfus	51.04	kJ/mol	Joback Method
hvap	78.95	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.556		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2199.30		NIST Webbook
rinpol	2199.30		NIST Webbook
tb	747.41	K	Joback Method
tc	922.67	K	Joback Method
tf	450.34	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.95	J/mol×K	747.41	Joback Method
cpg	798.88	J/mol×K	776.62	Joback Method
cpg	814.04	J/mol×K	805.83	Joback Method
cpg	828.48	J/mol×K	835.04	Joback Method
cpg	842.23	J/mol×K	864.25	Joback Method
cpg	855.32	J/mol×K	893.46	Joback Method
cpg	867.77	J/mol×K	922.67	Joback Method

hfust	54.20	kJ/mol	340.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57549e+01
Coeff. B	-6.33546e+03
Coeff. C	-1.37536e+02
Temperature range (K), min.	547.15
Temperature range (K), max.	744.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34450185&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

Legend

cpg:	Ideal gas heat capacity
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
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