15-methylhexadecanoic acid

Inchi: InChI=1S/C17H34O2/c1-16(2)14-12-10-8-6-4-3-5-7-9-11-13-15-17(18)19/h16H,3-15H2,1
InchiKey: IIUXHTGBZYEGHI-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CC(C)CCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 270.45
CAS: 1603-03-8

Physical Properties

Property code	Value	Unit	Source
gf	-175.92	kJ/mol	Joback Method
hf	-664.30	kJ/mol	Joback Method
hfus	41.95	kJ/mol	Joback Method
hvap	76.47	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.798		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
ripol	2980.00		NIST Webbook
ripol	2980.00		NIST Webbook
tb	733.97	K	Joback Method
tc	905.70	K	Joback Method
tf	377.10	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.57	J/mol×K	733.97	Joback Method
cpg	853.23	J/mol×K	877.08	Joback Method
cpg	839.56	J/mol×K	848.46	Joback Method
cpg	825.18	J/mol×K	819.83	Joback Method
cpg	810.08	J/mol×K	791.21	Joback Method
cpg	794.22	J/mol×K	762.59	Joback Method
cpg	866.23	J/mol×K	905.70	Joback Method

dvisc	0.0000272	Pa×s	733.97	Joback Method
dvisc	0.0000435	Pa×s	674.49	Joback Method
dvisc	0.0000762	Pa×s	615.01	Joback Method
dvisc	0.0001507	Pa×s	555.54	Joback Method
dvisc	0.0003509	Pa×s	496.06	Joback Method
dvisc	0.0010282	Pa×s	436.58	Joback Method
dvisc	0.0042295	Pa×s	377.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65953e+01
Coeff. B	-6.12828e+03
Coeff. C	-1.19529e+02
Temperature range (K), min.	495.32
Temperature range (K), max.	662.63

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=C1603038&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume