2-Ethylhexadecanoic acid

Inchi: InChI=1S/C18H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17(4-2)18(19)20/h17H,3-16H
InchiKey: YXLHBXPGRDAQSH-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCCCCCCCC(CC)C(=O)O
Mol. weight [g/mol]: 284.48
CAS: 54240-85-6

Physical Properties

Property code	Value	Unit	Source
gf	-167.50	kJ/mol	Joback Method
hf	-684.94	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	6.188		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	1979.00		NIST Webbook
rinpol	1979.00		NIST Webbook
tb	756.85	K	Joback Method
tc	930.87	K	Joback Method
tf	388.37	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.93	J/mol×K	756.85	Joback Method
cpg	913.77	J/mol×K	901.86	Joback Method
cpg	899.74	J/mol×K	872.86	Joback Method
cpg	884.97	J/mol×K	843.86	Joback Method
cpg	869.43	J/mol×K	814.86	Joback Method
cpg	853.09	J/mol×K	785.85	Joback Method
cpg	927.10	J/mol×K	930.87	Joback Method

dvisc	0.0000226	Pa×s	756.85	Joback Method
dvisc	0.0000360	Pa×s	695.44	Joback Method
dvisc	0.0000630	Pa×s	634.02	Joback Method
dvisc	0.0001241	Pa×s	572.61	Joback Method
dvisc	0.0002878	Pa×s	511.20	Joback Method
dvisc	0.0008398	Pa×s	449.78	Joback Method
dvisc	0.0034379	Pa×s	388.37	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67152e+01
Coeff. B	-6.28483e+03
Coeff. C	-1.23143e+02
Temperature range (K), min.	505.72
Temperature range (K), max.	674.26

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=C54240856&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume