2-Ethyloctadecanoic acid

Inchi: InChI=1S/C20H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(4-2)20(21)22/h19H
InchiKey: OHIOERKSFVRABL-UHFFFAOYSA-N
Formula: C20H40O2
SMILES: CCCCCCCCCCCCCCCCCC(CC)C(=O)O
Mol. weight [g/mol]: 312.53
CAS: 14276-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-150.66	kJ/mol	Joback Method
hf	-726.22	kJ/mol	Joback Method
hfus	49.72	kJ/mol	Joback Method
hvap	83.15	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.969		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook
tb	802.61	K	Joback Method
tc	983.28	K	Joback Method
tf	410.91	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.53	J/mol×K	802.61	Joback Method
cpg	973.79	J/mol×K	832.72	Joback Method
cpg	991.13	J/mol×K	862.83	Joback Method
cpg	1007.57	J/mol×K	892.94	Joback Method
cpg	1023.16	J/mol×K	923.06	Joback Method
cpg	1037.93	J/mol×K	953.17	Joback Method
cpg	1051.93	J/mol×K	983.28	Joback Method

dvisc	0.0022773	Pa×s	410.91	Joback Method
dvisc	0.0005614	Pa×s	476.19	Joback Method
dvisc	0.0001940	Pa×s	541.48	Joback Method
dvisc	0.0000842	Pa×s	606.76	Joback Method
dvisc	0.0000430	Pa×s	672.04	Joback Method
dvisc	0.0000247	Pa×s	737.33	Joback Method
dvisc	0.0000156	Pa×s	802.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73673e+01
Coeff. B	-6.79732e+03
Coeff. C	-1.31344e+02
Temperature range (K), min.	529.32
Temperature range (K), max.	695.16

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14276803&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

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