

2-Ethylotadecanoic 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:	CCCCCCCCCCCCCCCC(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
mvol	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	m ³ /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	Paxs	410.91	Joback Method
dvisc	0.0005614	Paxs	476.19	Joback Method
dvisc	0.0001940	Paxs	541.48	Joback Method
dvisc	0.0000842	Paxs	606.76	Joback Method
dvisc	0.0000430	Paxs	672.04	Joback Method
dvisc	0.0000247	Paxs	737.33	Joback Method
dvisc	0.0000156	Paxs	802.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14276803&Units=SI

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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