2-Eicosanol

Other names: 1-Methyl-1-nonadecanol
Inchi: InChI=1S/C20H42O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2)21/h20-21H,3
InchiKey: RHEVFAMQJMWLFS-UHFFFAOYSA-N
Formula: C20H42O
SMILES: CCCCCCCCCCCCCCCCCCC(C)O
Mol. weight [g/mol]: 298.55
CAS: 4340-76-5

Physical Properties

Property code	Value	Unit	Source
gf	-21.74	kJ/mol	Joback Method
hf	-613.64	kJ/mol	Joback Method
hfus	48.12	kJ/mol	Joback Method
hvap	76.41	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.019		Crippen Method
mcvol	298.530	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
tb	748.74	K	Joback Method
tc	918.70	K	Joback Method
tf	360.98	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.34	J/mol×K	748.74	Joback Method
cpg	1015.33	J/mol×K	890.37	Joback Method
cpg	999.36	J/mol×K	862.05	Joback Method
cpg	982.61	J/mol×K	833.72	Joback Method
cpg	965.04	J/mol×K	805.39	Joback Method
cpg	946.63	J/mol×K	777.07	Joback Method
cpg	1030.55	J/mol×K	918.70	Joback Method
dvisc	0.0000181	Pa×s	748.74	Joback Method

dvisc	0.0000299	Pa×s	684.11	Joback Method
dvisc	0.0000546	Pa×s	619.49	Joback Method
dvisc	0.0001147	Pa×s	554.86	Joback Method
dvisc	0.0002932	Pa×s	490.23	Joback Method
dvisc	0.0009971	Pa×s	425.61	Joback Method
dvisc	0.0052543	Pa×s	360.98	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59699e+01
Coeff. B	-5.95123e+03
Coeff. C	-1.18834e+02
Temperature range (K), min.	498.32
Temperature range (K), max.	677.19

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4340765&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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