9-Heptadecanol

Other names: 4-heptadecanol
Inchi: InChI=1S/C17H36O/c1-3-5-7-9-11-13-15-17(18)16-14-12-10-8-6-4-2/h17-18H,3-16H2,1-
InchiKey: WTWWTKPAEZQYPW-UHFFFAOYSA-N
Formula: C17H36O
SMILES: CCCCCCCCC(O)CCCCCCCC
Mol. weight [g/mol]: 256.47
CAS: 624-08-8

Physical Properties

Property code	Value	Unit	Source
gf	-47.00	kJ/mol	Joback Method
hf	-551.72	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	108.50 ± 0.40	kJ/mol	NIST Webbook
log10ws	-6.31		Crippen Method
logp	5.848		Crippen Method
mcvol	256.260	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
tb	680.10	K	Joback Method
tc	842.79	K	Joback Method
tf	311.50	K	Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	749.91	J/mol×K	680.10	Joback Method
cpg	767.57	J/mol×K	707.21	Joback Method
cpg	784.49	J/mol×K	734.33	Joback Method
cpg	800.68	J/mol×K	761.44	Joback Method
cpg	816.17	J/mol×K	788.56	Joback Method
cpg	830.98	J/mol×K	815.67	Joback Method
cpg	845.14	J/mol×K	842.79	Joback Method
dvisc	0.0107169	Pa×s	327.17	Joback Method
dvisc	0.0019407	Pa×s	385.99	Joback Method
dvisc	0.0005522	Pa×s	444.81	Joback Method
dvisc	0.0002108	Pa×s	503.63	Joback Method
dvisc	0.0000984	Pa×s	562.46	Joback Method
dvisc	0.0000531	Pa×s	621.28	Joback Method
dvisc	0.0000318	Pa×s	680.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59925e+01
Coeff. B	-5.63188e+03
Coeff. C	-1.07714e+02
Temperature range (K), min.	466.32
Temperature range (K), max.	634.99

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
Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7- and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
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=C624088&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
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