

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:	CCCCCCCCCC(O)CCCCCC
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
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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	Paxs	327.17	Joback Method
dvisc	0.0019407	Paxs	385.99	Joback Method
dvisc	0.0005522	Paxs	444.81	Joback Method
dvisc	0.0002108	Paxs	503.63	Joback Method
dvisc	0.0000984	Paxs	562.46	Joback Method
dvisc	0.0000531	Paxs	621.28	Joback Method
dvisc	0.0000318	Paxs	680.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the Joback Method: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, Mecitadecanol, 1-Eicosanol, Decacosanol, 1-Hexacosanol, and Cholesterofat 1) 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
	https://en.wikipedia.org/wiki/Joback_method
	http://link.springer.com/article/10.1007/BF02311772
	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

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