4-Octanol

Other names:	n-Octan-4-ol
	octan-4-ol
Inchi:	InChI=1S/C8H18O/c1-3-5-7-8(9)6-4-2/h8-9H,3-7H2,1-2H3
InchiKey:	WOFPPJOZXUTRAU-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(O)CCC
Mol. weight [g/mol]:	130.23
CAS:	589-62-8

Physical Properties

Property code	Value	Unit	Source
cpl	332.08	J/mol×K	Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols
gf	-122.78	kJ/mol	Joback Method
hf	-365.96	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	67.20 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.338		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rhoc	252.64	kg/m3	NIST Webbook
rhoc	252.64 ± 6.51	kg/m3	NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	977.00		NIST Webbook

rinpol	978.00		NIST Webbook
ripol	1376.00		NIST Webbook
tb	474.18	K	Joback Method
tc	625.10	K	NIST Webbook
tc	625.10 ± 0.30	K	NIST Webbook
tc	625.10 ± 0.50	K	NIST Webbook
tf	225.74	K	Joback Method
vc	0.515	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.23	J/mol×K	474.18	Joback Method
cpg	302.08	J/mol×K	501.33	Joback Method
cpg	313.47	J/mol×K	528.49	Joback Method
cpg	324.43	J/mol×K	555.64	Joback Method
cpg	334.96	J/mol×K	582.79	Joback Method
cpg	345.08	J/mol×K	609.94	Joback Method
cpg	354.79	J/mol×K	637.10	Joback Method
cpl	337.60	J/mol×K	298.50	NIST Webbook
dvisc	0.0169844	Pa×s	267.15	Joback Method
dvisc	0.1178389	Pa×s	225.74	Joback Method
dvisc	0.0041171	Pa×s	308.55	Joback Method
dvisc	0.0013956	Pa×s	349.96	Joback Method
dvisc	0.0005948	Pa×s	391.37	Joback Method
dvisc	0.0002984	Pa×s	432.77	Joback Method
dvisc	0.0001689	Pa×s	474.18	Joback Method
hvapt	57.30	kJ/mol	396.50	NIST Webbook
hvapt	54.80	kJ/mol	406.50	NIST Webbook
hvapt	62.10	kJ/mol	395.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62261e+01
Coeff. B	-4.02955e+03

Coeff. C	-9.69690e+01
Temperature range (K), min.	349.79
Temperature range (K), max.	466.16

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols:	https://www.doi.org/10.1016/j.jct.2006.10.007
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=C589628&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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