Pentane, 1-propoxy-

Other names: 1-propoxypentane

4-oxanonane

ether, pentyl propyl pentyl propyl ether propyl pentyl ether

InChl=1S/C8H18O/c1-3-5-6-8-9-7-4-2/h3-8H2,1-2H3

InchiKey: DMUSSSYUUUYJRM-UHFFFAOYSA-N

Formula: C8H18O

SMILES: CCCCCOCCC

Mol. weight [g/mol]: 130.23 CAS: 18641-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-88.52	kJ/mol	Joback Method
hf	-340.67	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	42.81	kJ/mol	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.603		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
рс	2492.52	kPa	Joback Method
tb	405.20	K	NIST Webbook
tc	568.81	K	Joback Method
tf	202.15	K	Joback Method
VC	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.91	J/mol×K	514.16	Joback Method
cpg	282.47	J/mol×K	459.51	Joback Method
cpg	270.17	J/mol×K	432.19	Joback Method
cpg	257.48	J/mol×K	404.86	Joback Method

cpg	317.06	J/mol×K	541.49	Joback Method	
cpg	327.83	J/mol×K	568.81	Joback Method	
cpg	294.38	J/mol×K	486.84	Joback Method	
dvisc	0.0017915	Paxs	235.94	Joback Method	
dvisc	0.0009546	Paxs	269.72	Joback Method	
dvisc	0.0005852	Paxs	303.50	Joback Method	
dvisc	0.0003956	Paxs	337.29	Joback Method	
dvisc	0.0002873	Paxs	371.08	Joback Method	
dvisc	0.0041498	Paxs	202.15	Joback Method	
dvisc	0.0002200	Paxs	404.86	Joback Method	
hvapt	35.00	kJ/mol	405.20	NIST Webbook	
rhol	742.73	kg/m3	323.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	
rhol	747.19	kg/m3	318.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	
rhol	756.01	kg/m3	308.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	
rhol	760.40	kg/m3	303.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	

rhol	764.78	kg/m3	298.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	
rhol	769.12	kg/m3	293.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	
rhol	773.45	kg/m3	288.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	
rhol	751.60	kg/m3	313.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model	

Sources

Crippen Method:

Liquid-liquid equilibrium in binary systems of isomeric C8 aliphatic (highelineliguidheniibhethainebinary systems of isomeric C8 aliphatic Excress fathalites aliphatic Excress fathalites aliphatic Excress fathalites and Their Description by the COSMO-SAC Model: McGowan Method:

NIST Webbook:

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

https://www.doi.org/10.1016/j.fluid.2013.07.002

https://www.doi.org/10.1016/j.jct.2014.12.025

https://www.doi.org/10.1021/acs.jced.5b00838

https://en.wikipedia.org/wiki/Joback_method

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

http://webbook.nist.gov/cgi/cbook.cgi?ID=C18641822&Units=SI

http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formationhf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditionshvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficientmcvol: McGowan's characteristic volume

pc: Critical Pressurerhol: Liquid Density

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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