Propanoic acid, hexyl ester

Other names:	1-Hexyl propionate
	Hexyl propanoate
	Hexyl propionate
	Propionic acid, hexyl ester
	n-Hexyl n-propionate
	n-Hexyl propionate
Inchi:	InChI=1S/C9H18O2/c1-3-5-6-7-8-11-9(10)4-2/h3-8H2,1-2H3
InchiKey:	GOKKOFHHJFGZHW-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCOC(=O)CC
Mol. weight [g/mol]:	158.24
CAS:	2445-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-473.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1079.95		NIST Webbook
rinpol	1100.99		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1114.00		NIST Webbook

rinpol	1088.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1114.00	NIST Webbook
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rinpol	1084.00	NIST Webbook
ripol	1326.00	NIST Webbook
ripol	1353.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1362.00	NIST Webbook
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ripol	1349.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1342.00		NIST Webbook
tb	463.15 ± 0.30	K	NIST Webbook
tb	458.65 ± 1.00	K	NIST Webbook
tc	655.29	K	Joback Method
tf	215.70 ± 0.50	K	NIST Webbook
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/mol×K	481.61	Joback Method
cpg	336.15	J/mol×K	510.56	Joback Method
cpg	348.92	J/mol×K	539.50	Joback Method
cpg	361.21	J/mol×K	568.45	Joback Method
cpg	373.04	J/mol×K	597.40	Joback Method
cpg	384.40	J/mol×K	626.35	Joback Method
cpg	395.29	J/mol×K	655.29	Joback Method
dvisc	0.0033103	Pa×s	263.35	Joback Method
dvisc	0.0016384	Pa×s	299.73	Joback Method
dvisc	0.0009442	Pa×s	336.10	Joback Method
dvisc	0.0006060	Pa×s	372.48	Joback Method
dvisc	0.0004209	Pa×s	408.86	Joback Method
dvisc	0.0003103	Pa×s	445.23	Joback Method

dvisc	0.0002395	Pa×s	481.61	Joback Method
pvap	0.02	kPa	280.70	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.02	kPa	278.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.03	kPa	283.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.03	kPa	285.80	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.04	kPa	288.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.10	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.14	kPa	303.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.14	kPa	303.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.20	kPa	308.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.28	kPa	313.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.40	kPa	318.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.54	kPa	323.40	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.68	kPa	326.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.76	kPa	328.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.86	kPa	330.60	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.00	kPa	333.30	Vapour pressures and enthalpies of vaporization of aliphatic esters

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46290e+01
Coeff. B	-3.91943e+03
Coeff. C	-6.71260e+01
Temperature range (K), min.	340.42
Temperature range (K), max.	487.78

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

Vapour pressures and enthalpies of vaporization of aliphatic esters: https://www.doi.org/10.1016/j.fluid.2012.08.003

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1115.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445763&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
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