Hexanoic acid, propyl ester

Other names:	Propyl caproate
	Propyl hexanoate
	n-Propyl n-hexanoate
	n-propyl hexanoate
Inchi:	InChI=1S/C9H18O2/c1-3-5-6-7-9(10)11-8-4-2/h3-8H2,1-2H3
InchiKey:	HTUIWRWYYVBCFT-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCC(=O)OCCC
Mol. weight [g/mol]:	158.24
CAS:	626-77-7

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	1077.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1091.00		NIST Webbook

rinpol	1094.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1093.00	NIST Webbook
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rinpol	1094.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1077.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1097.00	NIST Webbook
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rinpol	1114.00	NIST Webbook
rinpol	1061.00	NIST Webbook
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ripol	1320.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1326.00		NIST Webbook
tb	458.70 ± 2.00	K	NIST Webbook
tb	458.70 ± 1.00	K	NIST Webbook
tb	460.30 ± 0.30	K	NIST Webbook
tc	655.29	K	Joback Method
tf	199.20 ± 0.50	K	NIST Webbook
tf	204.50 ± 0.80	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	0.0016384	Pa×s	299.73	Joback Method
dvisc	0.0033103	Pa×s	263.35	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
hvapt	52.80	kJ/mol	354.50	NIST Webbook
hvapt	52.10	kJ/mol	354.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53528e+01
Coeff. B	-4.15873e+03
Coeff. C	-6.90720e+01
Temperature range (K), min.	345.12
Temperature range (K), max.	483.23

Sources

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=C626777&Units=SI
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

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
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
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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