Propyl octanoate

Other names:	Octanoic acid, propyl ester
	Propyl caprylate
	n-Propyl n-octanoate
	n-propyl octanoate
Inchi:	InChI=1S/C11H22O2/c1-3-5-6-7-8-9-11(12)13-10-4-2/h3-10H2,1-2H3
InchiKey:	IDHBLVYDNJDWNO-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCCC(=O)OCCC
Mol. weight [g/mol]:	186.29
CAS:	624-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-515.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1277.00		NIST Webbook

rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1508.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	499.58 ± 0.30	K	NIST Webbook
tb	497.90 ± 2.00	K	NIST Webbook
tc	698.36	K	Joback Method
tf	228.20 ± 0.80	K	NIST Webbook
tf	227.00 ± 0.50	K	NIST Webbook
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.39	J/mol×K	669.86	Joback Method
cpg	471.67	J/mol×K	641.36	Joback Method
cpg	458.41	J/mol×K	612.87	Joback Method
cpg	444.58	J/mol×K	584.37	Joback Method
cpg	430.19	J/mol×K	555.87	Joback Method
cpg	415.24	J/mol×K	527.37	Joback Method
cpg	496.57	J/mol×K	698.36	Joback Method
dvisc	0.0032030	Pa×s	285.89	Joback Method
dvisc	0.0002056	Pa×s	527.37	Joback Method

dvisc	0.0002689	Pa×s	487.12	Joback Method
dvisc	0.0003692	Pa×s	446.88	Joback Method
dvisc	0.0005398	Pa×s	406.63	Joback Method
dvisc	0.0008577	Pa×s	366.38	Joback Method
dvisc	0.0015281	Pa×s	326.14	Joback Method
hvapt	58.80	kJ/mol	421.50	NIST Webbook
hvapt	58.20	kJ/mol	384.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55685e+01
Coeff. B	-4.53255e+03
Coeff. C	-8.00250e+01
Temperature range (K), min.	376.64
Temperature range (K), max.	521.92

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C624135&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

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

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