Heptanoic acid, propyl ester

Other names: Propyl heptanoate
n-Propyl heptanoate
n-Propyl n-heptanoate
Inchi: InChI=1S/C10H20O2/c1-3-5-6-7-8-10(11)12-9-4-2/h3-9H2,1-2H3
InchiKey: UWZVPQKWYFZLLW-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCCCCC(=O)OCCC
Mol. weight [g/mol]: 172.26
CAS: 7778-87-2

Physical Properties

Property code	Value	Unit	Source
gf	-200.60	kJ/mol	Joback Method
hf	-494.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.910		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1177.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1174.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	481.09 ± 0.30	K	NIST Webbook
tb	479.60 ± 2.00	K	NIST Webbook
tc	676.79	K	Joback Method
tf	209.70 ± 0.80	K	NIST Webbook
tf	208.40 ± 0.50	K	NIST Webbook
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.11	J/mol×K	504.49	Joback Method
cpg	382.26	J/mol×K	533.21	Joback Method
cpg	395.89	J/mol×K	561.92	Joback Method
cpg	409.00	J/mol×K	590.64	Joback Method
cpg	421.59	J/mol×K	619.36	Joback Method
cpg	433.67	J/mol×K	648.08	Joback Method
cpg	445.25	J/mol×K	676.79	Joback Method
dvisc	0.0032806	Pa×s	274.62	Joback Method
dvisc	0.0015931	Pa×s	312.93	Joback Method
dvisc	0.0009057	Pa×s	351.24	Joback Method
dvisc	0.0005753	Pa×s	389.56	Joback Method
dvisc	0.0003964	Pa×s	427.87	Joback Method
dvisc	0.0002904	Pa×s	466.18	Joback Method
dvisc	0.0002230	Pa×s	504.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50485e+01
Coeff. B	-4.23654e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	361.92
Temperature range (K), max.	510.00

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7778872&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