Propyl undecanoate

Inchi: InChI=1S/C14H28O2/c1-3-5-6-7-8-9-10-11-12-14(15)16-13-4-2/h3-13H2,1-2H3
InchiKey: ILQYZJGHYZFJPP-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 228.37

Physical Properties

Property code	Value	Unit	Source
gf	-166.92	kJ/mol	Joback Method
hf	-577.09	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.470		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1571.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	596.01	K	Joback Method
tc	764.02	K	Joback Method
tf	319.70	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.02	J/mol×K	596.01	Joback Method
cpg	583.90	J/mol×K	624.01	Joback Method
cpg	600.10	J/mol×K	652.01	Joback Method
cpg	615.63	J/mol×K	680.02	Joback Method

cpg	630.49	J/mol×K	708.02	Joback Method
cpg	644.71	J/mol×K	736.02	Joback Method
cpg	658.29	J/mol×K	764.02	Joback Method
dvisc	0.0027735	Pa×s	319.70	Joback Method
dvisc	0.0012632	Pa×s	365.75	Joback Method
dvisc	0.0006860	Pa×s	411.80	Joback Method
dvisc	0.0004212	Pa×s	457.86	Joback Method
dvisc	0.0002827	Pa×s	503.91	Joback Method
dvisc	0.0002029	Pa×s	549.96	Joback Method
dvisc	0.0001532	Pa×s	596.01	Joback Method

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=U405140&Units=SI
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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