Undecanoic acid, propyl ester

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]: 228.38

Physical Properties

Property code	Value	Unit	Source
af	0.7621		Cheméo Relay (1.0)
hf	-652.94	kJ/mol	Cheméo Relay (1.0)
hfus	34.80	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-4.83		Cheméo Relay (1.0)
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	1571.00		NIST Webbook
rinpol	1576.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	537.55	K	Cheméo Relay (1.0)
tc	712.55	K	Cheméo Relay (1.0)
tf	257.71	K	Cheméo Relay (1.0)
vc	0.841	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405140&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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