Tridecanoic acid, propyl ester

Other names: Propyl tridecanoate
Inchi: InChI=1S/C16H32O2/c1-3-5-6-7-8-9-10-11-12-13-14-16(17)18-15-4-2/h3-15H2,1-2H3
InchiKey: OKLFWHUPMHZXAC-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 256.42

Physical Properties

Property code	Value	Unit	Source
gf	-150.08	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	641.77	K	Joback Method
tc	809.14	K	Joback Method
tf	342.24	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/mol×K	641.77	Joback Method
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method

dvisc	0.0001221	Pa×s	641.77	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method

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=U405141&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume