4-Pentenoic acid, 2-methyl-, undecyl ester

Inchi: InChI=1S/C17H32O2/c1-4-6-7-8-9-10-11-12-13-15-19-17(18)16(3)14-5-2/h5,16H,2,4,6-1
InchiKey: ZZYJIZQKVCIDKU-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-56.26	kJ/mol	Joback Method
hf	-518.86	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.273		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	1809.00		NIST Webbook
rinpol	1809.00		NIST Webbook
tb	660.89	K	Joback Method
tc	832.35	K	Joback Method
tf	336.75	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.23	J/mol×K	660.89	Joback Method
cpg	727.35	J/mol×K	689.47	Joback Method
cpg	744.65	J/mol×K	718.04	Joback Method
cpg	761.16	J/mol×K	746.62	Joback Method
cpg	776.89	J/mol×K	775.20	Joback Method
cpg	791.86	J/mol×K	803.77	Joback Method
cpg	806.10	J/mol×K	832.35	Joback Method
dvisc	0.0027986	Pa×s	336.75	Joback Method

dvisc	0.0011102	Pa×s	390.77	Joback Method
dvisc	0.0005513	Pa×s	444.80	Joback Method
dvisc	0.0003186	Pa×s	498.82	Joback Method
dvisc	0.0002050	Pa×s	552.84	Joback Method
dvisc	0.0001426	Pa×s	606.87	Joback Method
dvisc	0.0001053	Pa×s	660.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406114&Units=SI
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

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