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

Inchi: InChI=1S/C18H34O2/c1-4-6-7-8-9-10-11-12-13-14-16-20-18(19)17(3)15-5-2/h5,17H,2,4,
InchiKey: OCTXRPXMWDITBY-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-47.84	kJ/mol	Joback Method
hf	-539.50	kJ/mol	Joback Method
hfus	40.36	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.663		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	1907.00		NIST Webbook
rinpol	1907.00		NIST Webbook
tb	683.77	K	Joback Method
tc	855.40	K	Joback Method
tf	348.02	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.22	J/mol×K	683.77	Joback Method
cpg	784.74	J/mol×K	712.38	Joback Method
cpg	802.42	J/mol×K	740.98	Joback Method
cpg	819.26	J/mol×K	769.59	Joback Method
cpg	835.31	J/mol×K	798.19	Joback Method
cpg	850.57	J/mol×K	826.80	Joback Method
cpg	865.07	J/mol×K	855.40	Joback Method
dvisc	0.0025474	Pa×s	348.02	Joback Method

dvisc	0.0010012	Pa×s	403.98	Joback Method
dvisc	0.0004939	Pa×s	459.94	Joback Method
dvisc	0.0002840	Pa×s	515.89	Joback Method
dvisc	0.0001820	Pa×s	571.85	Joback Method
dvisc	0.0001263	Pa×s	627.81	Joback Method
dvisc	0.0000930	Pa×s	683.77	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=U406115&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume