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

Inchi: InChI=1S/C19H36O2/c1-4-6-7-8-9-10-11-12-13-14-15-17-21-19(20)18(3)16-5-2/h5,18H,2
InchiKey: QHJVHHWMUTUGCA-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 296.49

Physical Properties

Property code	Value	Unit	Source
gf	-39.42	kJ/mol	Joback Method
hf	-560.14	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	6.053		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	706.65	K	Joback Method
tc	878.93	K	Joback Method
tf	359.29	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.36	J/mol×K	706.65	Joback Method
cpg	843.28	J/mol×K	735.36	Joback Method
cpg	861.31	J/mol×K	764.08	Joback Method
cpg	878.48	J/mol×K	792.79	Joback Method
cpg	894.82	J/mol×K	821.50	Joback Method
cpg	910.34	J/mol×K	850.21	Joback Method
cpg	925.08	J/mol×K	878.93	Joback Method
dvisc	0.0023051	Pa×s	359.29	Joback Method

dvisc	0.0008981	Pa×s	417.18	Joback Method
dvisc	0.0004403	Pa×s	475.08	Joback Method
dvisc	0.0002520	Pa×s	532.97	Joback Method
dvisc	0.0001609	Pa×s	590.86	Joback Method
dvisc	0.0001113	Pa×s	648.76	Joback Method
dvisc	0.0000818	Pa×s	706.65	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=U406116&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