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

Inchi: InChI=1S/C20H38O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-18-22-20(21)19(3)17-5-2/h5,19
InchiKey: AITVUERWEKFFAB-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.51

Physical Properties

Property code	Value	Unit	Source
gf	-31.00	kJ/mol	Joback Method
hf	-580.78	kJ/mol	Joback Method
hfus	45.54	kJ/mol	Joback Method
hvap	68.21	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.443		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	729.53	K	Joback Method
tc	902.98	K	Joback Method
tf	370.56	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.57	J/mol×K	729.53	Joback Method
cpg	902.88	J/mol×K	758.44	Joback Method
cpg	921.27	J/mol×K	787.35	Joback Method
cpg	938.76	J/mol×K	816.26	Joback Method
cpg	955.38	J/mol×K	845.16	Joback Method
cpg	971.16	J/mol×K	874.07	Joback Method
cpg	986.12	J/mol×K	902.98	Joback Method
dvisc	0.0020748	Pa×s	370.56	Joback Method

dvisc	0.0008018	Pa×s	430.39	Joback Method
dvisc	0.0003908	Pa×s	490.22	Joback Method
dvisc	0.0002227	Pa×s	550.04	Joback Method
dvisc	0.0001417	Pa×s	609.87	Joback Method
dvisc	0.0000977	Pa×s	669.70	Joback Method
dvisc	0.0000717	Pa×s	729.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406117&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

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