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

Inchi: InChI=1S/C22H42O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-20-24-22(23)21(3)19-5-2
InchiKey: AFDKHYRYTRWOSQ-UHFFFAOYSA-N
Formula: C22H42O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 338.57

Physical Properties

Property code	Value	Unit	Source
gf	-14.16	kJ/mol	Joback Method
hf	-622.06	kJ/mol	Joback Method
hfus	50.72	kJ/mol	Joback Method
hvap	72.66	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	7.223		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	775.29	K	Joback Method
tc	952.90	K	Joback Method
tf	393.10	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.89	J/mol×K	775.29	Joback Method
cpg	1025.02	J/mol×K	804.89	Joback Method
cpg	1044.14	J/mol×K	834.49	Joback Method
cpg	1062.28	J/mol×K	864.09	Joback Method
cpg	1079.47	J/mol×K	893.69	Joback Method
cpg	1095.75	J/mol×K	923.30	Joback Method
cpg	1111.14	J/mol×K	952.90	Joback Method
dvisc	0.0016574	Pa×s	393.10	Joback Method

dvisc	0.0006309	Pa×s	456.80	Joback Method
dvisc	0.0003042	Pa×s	520.50	Joback Method
dvisc	0.0001719	Pa×s	584.19	Joback Method
dvisc	0.0001087	Pa×s	647.89	Joback Method
dvisc	0.0000746	Pa×s	711.59	Joback Method
dvisc	0.0000545	Pa×s	775.29	Joback Method

Sources

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=U406119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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