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

Inchi: InChI=1S/C21H40O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-19-23-21(22)20(3)18-5-2/h5
InchiKey: NQUFOCGJLQNROD-UHFFFAOYSA-N
Formula: C21H40O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 324.54

Physical Properties

Property code	Value	Unit	Source
gf	-22.58	kJ/mol	Joback Method
hf	-601.42	kJ/mol	Joback Method
hfus	48.13	kJ/mol	Joback Method
hvap	70.44	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.833		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	2214.00		NIST Webbook
tb	752.41	K	Joback Method
tc	927.62	K	Joback Method
tf	381.83	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.77	J/mol×K	752.41	Joback Method
cpg	963.48	J/mol×K	781.61	Joback Method
cpg	982.23	J/mol×K	810.81	Joback Method
cpg	1000.04	J/mol×K	840.01	Joback Method
cpg	1016.94	J/mol×K	869.21	Joback Method
cpg	1032.97	J/mol×K	898.42	Joback Method
cpg	1048.15	J/mol×K	927.62	Joback Method
dvisc	0.0018585	Pa×s	381.83	Joback Method
dvisc	0.0007126	Pa×s	443.59	Joback Method

dvisc	0.0003454	Pa×s	505.36	Joback Method
dvisc	0.0001960	Pa×s	567.12	Joback Method
dvisc	0.0001243	Pa×s	628.88	Joback Method
dvisc	0.0000856	Pa×s	690.65	Joback Method
dvisc	0.0000626	Pa×s	752.41	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=U406118&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