Pentadecanoic acid, 2,6,10,14-tetramethyl-, methyl ester

Other names: Pentadecanoic acid, 2,6,10,14-tetramethyl-, methyl ester, (2RS,6R,10R)-
2,6,10,14-Tetramethylpentadecanoic acid, methyl ester
Methyl nonadecanoate (isoprenoid)
Pristanic acid, methyl ester

Inchi: InChI=1S/C20H40O2/c1-16(2)10-7-11-17(3)12-8-13-18(4)14-9-15-19(5)20(21)22-6/h16-1

InchiKey: LCWYDFQCGCPILG-UHFFFAOYSA-N

Formula: C20H40O2

SMILES: COC(=O)C(C)CCCC(C)CCCC(C)CCCC(C)C

Mol. weight [g/mol]: 312.53

CAS: 1001-80-5

Physical Properties

Property code	Value	Unit	Source
gf	-126.16	kJ/mol	Joback Method
hf	-722.05	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	6.235		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
tb	731.53	K	Joback Method
tc	908.43	K	Joback Method
tf	327.32	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.24	J/mol×K	731.53	Joback Method
cpg	1002.33	J/mol×K	878.94	Joback Method
cpg	985.83	J/mol×K	849.46	Joback Method
cpg	968.39	J/mol×K	819.98	Joback Method
cpg	950.00	J/mol×K	790.50	Joback Method

cpg	930.62	J/mol×K	761.01	Joback Method
cpg	1017.92	J/mol×K	908.43	Joback Method
dvisc	0.0000532	Pa×s	731.53	Joback Method
dvisc	0.0000775	Pa×s	664.16	Joback Method
dvisc	0.0001229	Pa×s	596.79	Joback Method
dvisc	0.0002192	Pa×s	529.42	Joback Method
dvisc	0.0004628	Pa×s	462.06	Joback Method
dvisc	0.0012608	Pa×s	394.69	Joback Method
dvisc	0.0051894	Pa×s	327.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1001805&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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