Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Other names: Palmitin, 2-mono-
Palmitic acid «beta»-monoglyceride
2-Hexadecanoyl glycerol
2-Monopalmitin
2-Monopalmitoyl-sn-glycerol
Glycerol «beta»-palmitate
2-Hydroxy-1-(hydroxymethyl)ethyl palmitate
Glycerol 2-hexadecanoate
Glycerol, 2-palmitate
2-Monopalmitoylglycerol
2-Palmitoylglycerol
«beta»-Monopalmitin

Inchi: InChI=1S/C19H38O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19(22)23-18(16-20)17-21/h1

InchiKey: BBNYCLAREVXOSG-UHFFFAOYSA-N

Formula: C19H38O4

SMILES: CCCCCCCCCCCCCCCC(=O)OC(CO)CO

Mol. weight [g/mol]: 330.50

CAS: 23470-00-0

Physical Properties

Property code	Value	Unit	Source
chs	-11666.20 ± 2.80	kJ/mol	NIST Webbook
chs	-11685.30 ± 2.80	kJ/mol	NIST Webbook
gf	-400.90	kJ/mol	Joback Method
hf	-990.03	kJ/mol	Joback Method
hfs	-1222.10 ± 3.10	kJ/mol	NIST Webbook
hfs	-1239.80	kJ/mol	NIST Webbook
hfus	52.41	kJ/mol	Joback Method
hvap	100.01	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.364		Crippen Method
mcvol	297.750	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2519.30		NIST Webbook

rinpol	2519.30		NIST Webbook
tb	894.33	K	Joback Method
tc	1098.75	K	Joback Method
tf	482.69	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.19	J/mol×K	894.33	Joback Method
cpg	1013.04	J/mol×K	928.40	Joback Method
cpg	1028.81	J/mol×K	962.47	Joback Method
cpg	1043.52	J/mol×K	996.54	Joback Method
cpg	1057.22	J/mol×K	1030.61	Joback Method
cpg	1069.95	J/mol×K	1064.68	Joback Method
cpg	1081.75	J/mol×K	1098.75	Joback Method
cps	558.60	J/mol×K	298.00	NIST Webbook
cps	607.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0004753	Pa×s	482.69	Joback Method
dvisc	0.0001027	Pa×s	551.30	Joback Method
dvisc	0.0000311	Pa×s	619.90	Joback Method
dvisc	0.0000120	Pa×s	688.51	Joback Method
dvisc	0.0000055	Pa×s	757.12	Joback Method
dvisc	0.0000029	Pa×s	825.72	Joback Method
dvisc	0.0000016	Pa×s	894.33	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23470000&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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