Hexadecanoic acid, hexadecyl ester

Other names:	Cetin
	Crodamol CP
	Cutina CP
	Hexadecyl ester of hexadecanoic acid
	Hexadecyl palmitate
	Kessco 653
	Palmitic acid, cetyl ester
	Palmitic acid, hexadecyl ester
	Precifac ATO
	Radia 7500
	Rewowax CG
	Schercemol CP
	Standamul 1616
	Starfol CP
	Waxenol 815
	cetyl palmitate
	hexadecanoic acid, 1-hexadecyl ester
	hexadecyl hexadecanoate
	n-Hexadecyl hexadecanoate
	palmitic acid, palmityl ester
	palmityl palmitate
Inchi:	InChI=1S/C32H64O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-34-32(33)30-28-26-
InchiKey:	PXDJXZJSCPSGGI-UHFFFAOYSA-N
Formula:	C32H64O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCC
Mol. weight [g/mol]:	480.85
CAS:	540-10-3

Physical Properties

Property code	Value	Unit	Source
gf	-15.36	kJ/mol	Joback Method
hf	-948.61	kJ/mol	Joback Method
hfus	81.42	kJ/mol	Joback Method
hvap	95.98	kJ/mol	Joback Method
log10ws	-12.08		Crippen Method
logp	11.492		Crippen Method

mcvol	469.180	ml/mol	McGowan Method
pc	555.20	kPa	Joback Method
rinpol	3347.13		NIST Webbook
tb	1007.85	K	Joback Method
tc	1268.18	K	Joback Method
tf	314.42	K	Thermal analysis and quantitative characterization of compatibility between diflunisal and lipid excipients as raw materials for development of solid lipid nanoparticles
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1683.18	J/mol×K	1007.85	Joback Method
cpg	1803.68	J/mol×K	1224.79	Joback Method
cpg	1783.67	J/mol×K	1181.40	Joback Method
cpg	1761.76	J/mol×K	1138.01	Joback Method
cpg	1737.81	J/mol×K	1094.63	Joback Method
cpg	1711.67	J/mol×K	1051.24	Joback Method
cpg	1821.94	J/mol×K	1268.18	Joback Method
dvisc	0.0000123	Pa×s	1007.85	Joback Method
dvisc	0.0000169	Pa×s	926.97	Joback Method
dvisc	0.0000247	Pa×s	846.09	Joback Method
dvisc	0.0000392	Pa×s	765.20	Joback Method
dvisc	0.0000693	Pa×s	684.32	Joback Method
dvisc	0.0001429	Pa×s	603.44	Joback Method
dvisc	0.0003683	Pa×s	522.56	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermal analysis and quantitative characterization of compatibility between diflunisal and lipid excipients as raw materials for development of solid lipid nanoparticles: https://www.doi.org/10.1016/j.tca.2016.09.014

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=C540103&Units=SI

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