Octadecanoic acid, hexadecyl ester

Other names:	Octadecanoic acid, hexadecyl ester
	Stearic acid, hexadecyl ester
	Hexadecyl octadecanoate
	Hexadecyl stearate
	Wickenol 121
	n-Hexadecyl stearate
	Schercemol CS
	Palmityl stearate
Inchi:	InChI=1S/C34H68O2/c1-3-5-7-9-11-13-15-17-19-20-22-24-26-28-30-32-34(35)36-33-31-
InchiKey:	SSZBUIDZHHWXNJ-UHFFFAOYSA-N
Formula:	C34H68O2
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	508.92

Physical Properties

Property code	Value	Unit	Source
af	1.4663		Cheméo Relay (1.0)
hf	-1060.95	kJ/mol	Cheméo Relay (1.0)
hfus	86.60	kJ/mol	Joback Method
hvap	157.96	kJ/mol	Cheméo Relay (1.0)
ie	10.12	eV	Cheméo Relay (1.0)
log10ws	-10.82		Cheméo Relay (1.0)
logp	12.272		Crippen Method
mcvol	497.360	ml/mol	McGowan Method
pc	508.18	kPa	Joback Method
rinpol	3546.45		NIST Webbook
tb	682.15	K	Cheméo Relay (1.0)
tc	865.19	K	Cheméo Relay (1.0)
tf	330.00 ± 0.50	K	NIST Webbook
vc	1.957	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1818.58	J/mol×K	1053.61	Joback Method
cpg	1849.65	J/mol×K	1102.55	Joback Method
cpg	1877.82	J/mol×K	1151.48	Joback Method
cpg	1903.31	J/mol×K	1200.42	Joback Method
cpg	1926.37	J/mol×K	1249.35	Joback Method
cpg	1947.21	J/mol×K	1298.29	Joback Method
cpg	1966.09	J/mol×K	1347.22	Joback Method
dvisc	0.0002762	Pa×s	545.10	Joback Method
dvisc	0.0001060	Pa×s	629.85	Joback Method
dvisc	0.0000510	Pa×s	714.60	Joback Method
dvisc	0.0000287	Pa×s	799.36	Joback Method
dvisc	0.0000180	Pa×s	884.11	Joback Method
dvisc	0.0000123	Pa×s	968.86	Joback Method
dvisc	0.0000089	Pa×s	1053.61	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1190632&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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