Octadecanoic acid, eicosyl ester

Other names:	Stearic acid, eicosyl ester
	Eicosyl stearate
	icosyl stearate
	eicosanyl octadecanoate
Inchi:	InChI=1S/C38H76O2/c1-3-5-7-9-11-13-15-17-19-20-21-23-25-27-29-31-33-35-37-40-38(
InchiKey:	SOCXDNMHDNVKIL-UHFFFAOYSA-N
Formula:	C38H76O2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	565.01
CAS:	22413-02-1

Physical Properties

Property code	Value	Unit	Source
gf	35.16	kJ/mol	Joback Method
hf	-1072.45	kJ/mol	Joback Method
hfus	96.96	kJ/mol	Joback Method
hvap	109.34	kJ/mol	Joback Method
log10ws	-14.59		Crippen Method
logp	13.833		Crippen Method
mcvol	553.720	ml/mol	McGowan Method
pc	430.43	kPa	Joback Method
rinpol	3946.15		NIST Webbook
tb	1145.13	K	Joback Method
tc	1530.59	K	Joback Method
tf	590.18	K	Joback Method
vc	2.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2091.96	J/mol×K	1145.13	Joback Method
cpg	2129.57	J/mol×K	1209.37	Joback Method
cpg	2162.67	J/mol×K	1273.62	Joback Method
cpg	2191.88	J/mol×K	1337.86	Joback Method

cpg	2217.78	J/mol×K	1402.10	Joback Method
cpg	2240.98	J/mol×K	1466.35	Joback Method
cpg	2262.08	J/mol×K	1530.59	Joback Method
dvisc	0.0001520	Pa×s	590.18	Joback Method
dvisc	0.0000572	Pa×s	682.67	Joback Method
dvisc	0.0000272	Pa×s	775.16	Joback Method
dvisc	0.0000151	Pa×s	867.66	Joback Method
dvisc	0.0000094	Pa×s	960.15	Joback Method
dvisc	0.0000064	Pa×s	1052.64	Joback Method
dvisc	0.0000046	Pa×s	1145.13	Joback Method

Sources

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=C22413021&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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