Dodecanoic acid, octadecyl ester

Other names:	Lauric acid, octadecyl ester
	Octadecyl dodecanoate
	Octadecyl laurate
	Stearyl laurate
Inchi:	InChI=1S/C30H60O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-27-29-32-30(31)28-
InchiKey:	TZXYSEYEGNHPQI-UHFFFAOYSA-N
Formula:	C30H60O2
SMILES:	CCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	452.80
CAS:	3234-84-2

Physical Properties

Property code	Value	Unit	Source
gf	-32.20	kJ/mol	Joback Method
hf	-907.33	kJ/mol	Joback Method
hfus	76.24	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-11.24		Crippen Method
logp	10.712		Crippen Method
mcvol	441.000	ml/mol	McGowan Method
pc	609.06	kPa	Joback Method
rinpol	3150.85		NIST Webbook
tb	962.09	K	Joback Method
tc	1195.84	K	Joback Method
tf	500.02	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.95	J/mol×K	962.09	Joback Method
cpg	1662.31	J/mol×K	1156.88	Joback Method
cpg	1643.07	J/mol×K	1117.92	Joback Method
cpg	1622.22	J/mol×K	1078.97	Joback Method

cpg	1599.65	J/mol×K	1040.01	Joback Method
cpg	1575.26	J/mol×K	1001.05	Joback Method
cpg	1680.03	J/mol×K	1195.84	Joback Method
dvisc	0.0000168	Pa×s	962.09	Joback Method
dvisc	0.0000231	Pa×s	885.08	Joback Method
dvisc	0.0000337	Pa×s	808.07	Joback Method
dvisc	0.0000532	Pa×s	731.05	Joback Method
dvisc	0.0000936	Pa×s	654.04	Joback Method
dvisc	0.0001913	Pa×s	577.03	Joback Method
dvisc	0.0004872	Pa×s	500.02	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3234842&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
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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