

Octadecanoic acid, docosyl ester

Other names:	Stearic acid, docosyl ester Docosyl stearate docosanyl octadecanoate
Inchi:	InChI=1S/C40H80O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-23-25-27-29-31-33-35-37-39-
InchiKey:	SRKUMCYSWLWLLS-UHFFFAOYSA-N
Formula:	C40H80O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	593.06
CAS:	22413-03-2

Physical Properties

Property code	Value	Unit	Source
gf	52.00	kJ/mol	Joback Method
hf	-1113.73	kJ/mol	Joback Method
hfus	102.14	kJ/mol	Joback Method
hvap	113.79	kJ/mol	Joback Method
log10ws	-15.43		Crippen Method
logp	14.613		Crippen Method
mcvol	581.900	ml/mol	McGowan Method
pc	398.09	kPa	Joback Method
rinpol	4146.65		NIST Webbook
rinpol	4146.65		NIST Webbook
tb	1190.89	K	Joback Method
tc	1638.25	K	Joback Method
tf	612.72	K	Joback Method
vc	2.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2229.58	J/molxK	1190.89	Joback Method
cpg	2271.31	J/molxK	1265.45	Joback Method
cpg	2307.48	J/molxK	1340.01	Joback Method
cpg	2339.08	J/molxK	1414.57	Joback Method

cpg	2367.11	J/molxK	1489.13	Joback Method
cpg	2392.58	J/molxK	1563.69	Joback Method
cpg	2416.46	J/molxK	1638.25	Joback Method
dvisc	0.0001118	Paxs	612.72	Joback Method
dvisc	0.0000417	Paxs	709.08	Joback Method
dvisc	0.0000197	Paxs	805.44	Joback Method
dvisc	0.0000109	Paxs	901.80	Joback Method
dvisc	0.0000068	Paxs	998.17	Joback Method
dvisc	0.0000046	Paxs	1094.53	Joback Method
dvisc	0.0000033	Paxs	1190.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22413032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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