1,2-Diaceto-3-stearin

Other names:	1,2-Diaceto-3-stearin
	2,3-Bis(acetyloxy)propyl stearate
	Glycerol, 1-octadecanoate, diacetate
	NSC 83201
	Stearic acid, 2,3-dihydroxypropyl ester diacetate
Inchi:	InChI=1S/C25H46O6/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-25(28)30-21-24(31
InchiKey:	WSYNAKWAAXYNMW-UHFFFAOYSA-N
Formula:	C25H46O6
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]:	442.63
CAS:	26836-44-2

Physical Properties

Property code	Value	Unit	Source
af	1.2286		Cheméo Relay (1.0)
hf	-1476.68	kJ/mol	Cheméo Relay (1.0)
hfus	65.34	kJ/mol	Joback Method
hvap	138.30	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	Cheméo Relay (1.0)
log10ws	-6.17		Cheméo Relay (1.0)
logp	6.286		Crippen Method
mcvol	385.430	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
tb	654.73	K	Cheméo Relay (1.0)
tc	820.23	K	Cheméo Relay (1.0)
tf	308.00 ± 0.20	K	NIST Webbook
tf	308.00 ± 0.20	K	NIST Webbook
vc	1.483	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.71	J/mol×K	1194.92	Joback Method
cpg	1412.30	J/mol×K	1233.94	Joback Method

cpg	1350.36	J/mol×K	1038.85	Joback Method
cpg	1366.61	J/mol×K	1077.87	Joback Method
cpg	1380.90	J/mol×K	1116.88	Joback Method
cpg	1393.25	J/mol×K	1155.90	Joback Method
cpg	1332.11	J/mol×K	999.83	Joback Method
cps	904.20	J/mol×K	298.20	NIST Webbook
dvisc	0.0000714	Pa×s	715.27	Joback Method
dvisc	0.0001286	Pa×s	644.13	Joback Method
dvisc	0.0002679	Pa×s	572.99	Joback Method
dvisc	0.0000441	Pa×s	786.41	Joback Method
dvisc	0.0000295	Pa×s	857.55	Joback Method
dvisc	0.0000210	Pa×s	928.69	Joback Method
dvisc	0.0000157	Pa×s	999.83	Joback Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26836442&Units=SI

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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

cps: Solid phase 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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume