Docosanoic acid, 1,2,3-propanetriyl ester

Other names:	Docosanoin, tri-
	Glyceryl behenate
	Tribehenin
	Glyceryl tribehenate
	Syncrowax HR-C
	propane-1,2,3-triyl tridocosanoate
Inchi:	InChI=1S/C69H134O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-55-58-61-
InchiKey:	DMBUODUULYCPAK-UHFFFAOYSA-N
Formula:	C69H134O6
SMILES:	CCCCCCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	1059.80
CAS:	18641-57-1

Physical Properties

Property code	Value	Unit	Source
chs	-43208.20 ± 1.80	kJ/mol	NIST Webbook
gf	-174.10	kJ/mol	Joback Method
hf	-2207.17	kJ/mol	Joback Method
hfus	179.30	kJ/mol	Joback Method
hvap	196.27	kJ/mol	Joback Method
log10ws	-25.40		Crippen Method
logp	23.450		Crippen Method
mcvol	1005.390	ml/mol	McGowan Method
pc	168.84	kPa	Joback Method
tb	2006.55	K	Joback Method
tf	1068.87	K	Joback Method
tt	340.60 ± 1.00	K	NIST Webbook
tt	346.50 ± 1.00	K	NIST Webbook
tt	355.50 ± 1.00	K	NIST Webbook
vc	3.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	4189.00	J/mol×K	2006.55	Joback Method
dvisc	0.0000002	Pa×s	1068.87	Joback Method
dvisc	8.6508315e-08	Pa×s	1225.15	Joback Method
dvisc	4.1518222e-08	Pa×s	1381.43	Joback Method
dvisc	2.3132569e-08	Pa×s	1537.71	Joback Method
dvisc	1.4357458e-08	Pa×s	1693.99	Joback Method
dvisc	9.6588133e-09	Pa×s	1850.27	Joback Method
dvisc	6.9117237e-09	Pa×s	2006.55	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C18641571&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point
tt: Triple Point Temperature
vc: Critical Volume

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