Decanoic acid, 2,3-dihydroxypropyl ester

Other names:	1-Monocaprin
	2,3-dihydroxypropyl decanoate
	Capric acid «alpha»-monoglyceride
	Decanoic acid 1-monoglyceride
	Decanoin, 1-mono-
	Glycerol 1-monodecanoate
	rac-Glycerol 1-monodecanoate
	«alpha»-Monocaprin
Inchi:	InChI=1S/C13H26O4/c1-2-3-4-5-6-7-8-9-13(16)17-11-12(15)10-14/h12,14-15H,2-11H2,1
InchiKey:	LKUNXBRZDFMZOK-UHFFFAOYSA-N
Formula:	C13H26O4
SMILES:	CCCCCCCCCC(=O)OCC(O)CO
Mol. weight [g/mol]:	246.34
CAS:	2277-23-8

Physical Properties

Property code	Value	Unit	Source
chs	-7722.50 ± 1.30	kJ/mol	NIST Webbook
gf	-451.42	kJ/mol	Joback Method
hf	-866.19	kJ/mol	Joback Method
hfs	-1109.00 ± 1.50	kJ/mol	NIST Webbook
hfus	36.87	kJ/mol	Joback Method
hvap	86.66	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.024		Crippen Method
mcvol	213.210	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	757.05	K	Joback Method
tc	930.94	K	Joback Method
tf	415.07	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.54	J/mol×K	901.96	Joback Method
cpg	683.16	J/mol×K	844.00	Joback Method
cpg	671.55	J/mol×K	815.01	Joback Method
cpg	659.30	J/mol×K	786.03	Joback Method
cpg	646.41	J/mol×K	757.05	Joback Method
cpg	714.34	J/mol×K	930.94	Joback Method
cpg	694.15	J/mol×K	872.98	Joback Method
cps	410.00	J/mol×K	298.00	NIST Webbook
dvisc	0.0004662	Pa×s	472.07	Joback Method
dvisc	0.0001366	Pa×s	529.06	Joback Method
dvisc	0.0000508	Pa×s	586.06	Joback Method
dvisc	0.0000225	Pa×s	643.06	Joback Method
dvisc	0.0000114	Pa×s	700.05	Joback Method
dvisc	0.0022293	Pa×s	415.07	Joback Method
dvisc	0.0000064	Pa×s	757.05	Joback Method
pvap	13.20	kPa	524.41	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	10.10	kPa	519.10	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	6.80	kPa	511.21	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	4.30	kPa	501.31	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique

pvap	3.60	kPa	498.31	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	3.10	kPa	497.13	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	2.50	kPa	491.77	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	1.50	kPa	482.79	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	1.10	kPa	478.69	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2277238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique:	https://www.doi.org/10.1021/je401080p

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume