

Decanoic acid, 2,3-dihydroxypropyl ester

Other names:	1-Monocaprin 2,3-dihydroxypropyl decanoate Capric acid «alpha»-monoglyceride Decanoic acid 1-monoglyceride Decanoïn, 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:	CCCCCCCCC(=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	646.41	J/molxK	757.05	Joback Method
cpg	659.30	J/molxK	786.03	Joback Method
cpg	671.55	J/molxK	815.01	Joback Method
cpg	683.16	J/molxK	844.00	Joback Method
cpg	694.15	J/molxK	872.98	Joback Method
cpg	704.54	J/molxK	901.96	Joback Method
cpg	714.34	J/molxK	930.94	Joback Method
cps	410.00	J/molxK	298.00	NIST Webbook
dvisc	0.0000064	Paxs	757.05	Joback Method
dvisc	0.0004662	Paxs	472.07	Joback Method
dvisc	0.0001366	Paxs	529.06	Joback Method
dvisc	0.0000508	Paxs	586.06	Joback Method
dvisc	0.0022293	Paxs	415.07	Joback Method
dvisc	0.0000114	Paxs	700.05	Joback Method
dvisc	0.0000225	Paxs	643.06	Joback Method
pvap	1.10	kPa	478.69	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	2.50	kPa	491.77	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	3.60	kPa	498.31	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	6.80	kPa	511.21	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	13.20	kPa	524.41	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique

Sources

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=C2277238&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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>

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

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