

1,3-Dioctanoin

Other names:	2-hydroxypropane-1,3-diyl dioctanoate glycerol 1,3-dicaprylate octanoic acid, 1,1'-(2-hydroxy-1,3-propanediyl) ester
Inchi:	InChI=1S/C19H36O5/c1-3-5-7-9-11-13-18(21)23-15-17(20)16-24-19(22)14-12-10-8-6-4-2
InchiKey:	DMPAVJVECSKEPF-UHFFFAOYSA-N
Formula:	C19H36O5
SMILES:	CCCCCCCC(=O)OCC(O)COC(=O)CCCCCCC
Mol. weight [g/mol]:	344.49
CAS:	1429-66-9

Physical Properties

Property code	Value	Unit	Source
gf	-498.00	kJ/mol	Joback Method
hf	-1082.60	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	92.49	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.155		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2375.70		NIST Webbook
rinpol	2375.70		NIST Webbook
tb	878.44	K	Joback Method
tc	1075.60	K	Joback Method
tf	494.03	K	Joback Method
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.17	J/mol×K	878.44	Joback Method
cpg	1060.34	J/mol×K	1075.60	Joback Method
cpg	1010.59	J/mol×K	944.16	Joback Method
cpg	1024.63	J/mol×K	977.02	Joback Method

cpg	1037.59	J/molxK	1009.88	Joback Method
cpg	1049.49	J/molxK	1042.74	Joback Method
cpg	995.44	J/molxK	911.30	Joback Method
dvisc	0.0000126	Paxs	814.37	Joback Method
dvisc	0.0000203	Paxs	750.30	Joback Method
dvisc	0.0000360	Paxs	686.24	Joback Method
dvisc	0.0000717	Paxs	622.17	Joback Method
dvisc	0.0001674	Paxs	558.10	Joback Method
dvisc	0.0000083	Paxs	878.44	Joback Method
dvisc	0.0004866	Paxs	494.03	Joback Method
pvap	10.10	kPa	560.35	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	13.20	kPa	567.73	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	6.80	kPa	552.59	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	4.30	kPa	541.18	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	3.10	kPa	533.36	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique

pvap	2.50	kPa	529.42	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	1.50	kPa	517.23	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	1.10	kPa	511.93	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	3.60	kPa	538.14	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=C1429669&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

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
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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