

1,3-Dicaprin

Other names:	(3-decanoyloxy-2-hydroxypropyl) decanoate 2-hydroxypropane-1,3-diyl bis(decanoate)
Inchi:	InChI=1S/C23H44O5/c1-3-5-7-9-11-13-15-17-22(25)27-19-21(24)20-28-23(26)18-16-14-
InchiKey:	BPYWNJQNVNYQSQ-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCCCC(=O)OCC(O)COC(=O)CCCCCCCC
Mol. weight [g/mol]:	400.59
CAS:	17598-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-464.32	kJ/mol	Joback Method
hf	-1165.16	kJ/mol	Joback Method
hfus	61.46	kJ/mol	Joback Method
hvap	101.39	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.715		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpola	2774.10		NIST Webbook
rinpola	2774.10		NIST Webbook
tb	969.96	K	Joback Method
tc	1198.35	K	Joback Method
tf	539.11	K	Joback Method
vc	1.385	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.37	J/mol×K	969.96	Joback Method
cpg	1243.95	J/mol×K	1008.03	Joback Method
cpg	1260.89	J/mol×K	1046.09	Joback Method
cpg	1276.24	J/mol×K	1084.16	Joback Method
cpg	1290.04	J/mol×K	1122.22	Joback Method

cpg	1302.35	J/molxK	1160.29	Joback Method
cpg	1313.21	J/molxK	1198.35	Joback Method
dvisc	0.0000039	Paxs	969.96	Joback Method
dvisc	0.0000798	Paxs	610.92	Joback Method
dvisc	0.0000339	Paxs	682.73	Joback Method
dvisc	0.0002359	Paxs	539.11	Joback Method
dvisc	0.0000096	Paxs	826.34	Joback Method
dvisc	0.0000059	Paxs	898.15	Joback Method
dvisc	0.0000170	Paxs	754.53	Joback Method
pvap	1.00	kPa	535.66	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	1.10	kPa	538.32	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	1.50	kPa	544.06	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	2.50	kPa	554.25	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	3.10	kPa	558.74	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique

pvap	3.60	kPa	562.37	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique
pvap	4.30	kPa	565.39	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=C17598935&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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

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