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: CCCCCCCCCC(=O)OCC(O)COC(=O)CCCCCCCCC
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
rinpol	2774.10		NIST Webbook
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.21	J/mol×K	1198.35	Joback Method
cpg	1290.04	J/mol×K	1122.22	Joback Method
cpg	1276.24	J/mol×K	1084.16	Joback Method
cpg	1260.89	J/mol×K	1046.09	Joback Method
cpg	1243.95	J/mol×K	1008.03	Joback Method

cpg	1225.37	J/mol×K	969.96	Joback Method
cpg	1302.35	J/mol×K	1160.29	Joback Method
dvisc	0.0000798	Pa×s	610.92	Joback Method
dvisc	0.0000339	Pa×s	682.73	Joback Method
dvisc	0.0000170	Pa×s	754.53	Joback Method
dvisc	0.0000096	Pa×s	826.34	Joback Method
dvisc	0.0000059	Pa×s	898.15	Joback Method
dvisc	0.0002359	Pa×s	539.11	Joback Method
dvisc	0.0000039	Pa×s	969.96	Joback Method
pvap	4.30	kPa	565.39	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	3.10	kPa	558.74	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	1.50	kPa	544.06	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	1.00	kPa	535.66	Boiling Points of Short-Chain Partial Acylglycerols and Tocopherols at Low Pressures by the Differential Scanning Calorimetry Technique

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17598935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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