

1,2-Dicaprin

Inchi:	InChI=1S/C23H44O5/c1-3-5-7-9-11-13-15-17-22(25)27-20-21(19-24)28-23(26)18-16-14-
InchiKey:	GNSDEDOVXZDMKM-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCCCC(=O)OCC(CO)OC(=O)CCCCCCCC
Mol. weight [g/mol]:	400.59
CAS:	17863-69-3

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	2752.70		NIST Webbook
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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/mol×K	1160.29	Joback Method
cpg	1313.21	J/mol×K	1198.35	Joback Method

dvisc	0.0002359	Paxs	539.11	Joback Method
dvisc	0.0000798	Paxs	610.92	Joback Method
dvisc	0.0000339	Paxs	682.73	Joback Method
dvisc	0.0000170	Paxs	754.53	Joback Method
dvisc	0.0000096	Paxs	826.34	Joback Method
dvisc	0.0000059	Paxs	898.15	Joback Method
dvisc	0.0000039	Paxs	969.96	Joback Method

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=C17863693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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