

L-Serine, N,O-bis(capryloyl)-, methyl ester

Inchi: InChI=1S/C20H37NO5/c1-4-6-8-10-12-14-18(22)21-17(20(24)25-3)16-26-19(23)15-13-1
InchiKey: DXUOHGDEBRLPEU-UHFFFAOYSA-N
Formula: C20H37NO5
SMILES: CCCCCCCC(=O)OCC(N=C(O)CCCCCCC)C(=O)OC
Mol. weight [g/mol]: 371.51

Physical Properties

Property code	Value	Unit	Source
hf	-1030.81	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.749		Crippen Method
mcvol	319.090	ml/mol	McGowan Method
pc	1077.81	kPa	Joback Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
tb	977.88	K	Joback Method
tc	1199.89	K	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=U299729&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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