Pentanedioic acid, 2-octanoylamino, dimethyl ester

Inchi: InChI=1S/C15H27NO5/c1-4-5-6-7-8-9-13(17)16-12(15(19)21-3)10-11-14(18)20-2/h12H,4

InchiKey: GKNLUTKJUBKURO-UHFFFAOYSA-N

Formula: C15H27NO5

SMILES: CCCCCCCC(O)=NC(CCC(=O)OC)C(=O)OC

Mol. weight [g/mol]: 301.38

Physical Properties

Property code	Value	Unit	Source
hf	-927.61	kJ/mol	Joback Method
hvap	86.98	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.798		Crippen Method
mcvol	248.640	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	863.48	K	Joback Method
tc	1060.61	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=R106664&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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