DL-2-Aminoadipic acid, N-dimethylaminomethylene-, dibutyl ester

Inchi: InChI=1S/C17H32N2O4/c1-5-7-12-22-16(20)11-9-10-15(18-14-19(3)4)17(21)23-13-8-6-2

InchiKey: UEDWUWJAAVUUBK-UHFFFAOYSA-N

Formula: C17H32N2O4

SMILES: CCCCOC(=O)CCCC(N=CN(C)C)C(=O)OCCCC

Mol. weight [g/mol]: 328.45

Physical Properties

Property code	Value	Unit	Source
hf	-739.34	kJ/mol	Joback Method
hvap	76.72	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.802		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	2204.00		NIST Webbook
tb	829.62	K	Joback Method
tc	1022.67	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375709&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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