Carbonic acid, monoamide, N-hexadecyl-, decyl ester

Inchi: InChI=1S/C27H55NO2/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-28-27(29)30-26-24

InchiKey: HULDRIDDDNECTJ-UHFFFAOYSA-N

Formula: C27H55NO2

SMILES: CCCCCCCCCCCCCCCCCN=C(O)OCCCCCCCCCC

Mol. weight [g/mol]: 425.73

Physical Properties

Property code	Value	Unit	Source
hf	-812.63	kJ/mol	Joback Method
hvap	98.18	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	9.539		Crippen Method
mcvol	408.710	ml/mol	McGowan Method
pc	679.94	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
tb	1008.32	K	Joback Method
tc	1259.49	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415189&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