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

Inchi: InChI=1S/C22H45NO2/c1-3-5-7-9-11-13-14-16-18-20-23-22(24)25-21-19-17-15-12-10-8-

InchiKey: AQRPIQIQCMISKD-UHFFFAOYSA-N

Formula: C22H45NO2

SMILES: CCCCCCCCCCCN=C(O)OCCCCCCCCCC

Mol. weight [g/mol]: 355.60

Physical Properties

Property code	Value	Unit	Source
hf	-709.43	kJ/mol	Joback Method
hvap	87.05	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.588		Crippen Method
mcvol	338.260	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	2927.00		NIST Webbook
rinpol	2927.00		NIST Webbook
tb	893.92	K	Joback Method
tc	1095.86	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415186&Units=SI

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

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