Carbonic acid, monoamide, N-hept-2-yl-, decyl ester

Inchi: InChI=1S/C18H37NO2/c1-4-6-8-9-10-11-12-14-16-21-18(20)19-17(3)15-13-7-5-2/h17H,4

InchiKey: KIWNUJQLPAGGFD-UHFFFAOYSA-N

Formula: C18H37NO2

SMILES: CCCCCCCCCCOC(O)=NC(C)CCCCC

Mol. weight [g/mol]: 299.49

Physical Properties

Property code	Value	Unit	Source
hf	-632.15	kJ/mol	Joback Method
hvap	77.76	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	6.027		Crippen Method
mcvol	281.900	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	801.96	K	Joback Method
tc	984.84	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415179&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