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

Inchi: InChI=1S/C20H41NO2/c1-3-5-7-9-11-12-13-14-16-18-21-20(22)23-19-17-15-10-8-6-4-2/h

InchiKey: ZJIBREGPWJRAKD-UHFFFAOYSA-N

Formula: C20H41NO2

SMILES: CCCCCCCCCCCN=C(O)OCCCCCCCC

Mol. weight [g/mol]: 327.55

Physical Properties

Property code	Value	Unit	Source
hf	-668.15	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.808		Crippen Method
mcvol	310.080	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	848.16	K	Joback Method
tc	1038.42	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U406544&Units=SI

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