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

Inchi: InChI=1S/C21H43NO2/c1-3-5-7-9-11-12-13-14-15-17-19-22-21(23)24-20-18-16-10-8-6-4

InchiKey: WNSSHFYWVJLCIE-UHFFFAOYSA-N

Formula: C21H43NO2

SMILES: CCCCCCCCCCCCN=C(O)OCCCCCCCC

Mol. weight [g/mol]: 341.57

Physical Properties

Property code	Value	Unit	Source
hf	-688.79	kJ/mol	Joback Method
hvap	84.82	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	7.198		Crippen Method
mcvol	324.170	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	871.04	K	Joback Method
tc	1066.65	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U406574&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

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