

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

Inchi:	InChI=1S/C18H37NO2/c1-3-5-7-9-10-11-12-13-14-16-19-18(20)21-17-15-8-6-4-2/h3-17H
InchiKey:	HELBJERRLLLYHC-UHFFFAOYSA-N
Formula:	C18H37NO2
SMILES:	CCCCCCCCCCCN=C(O)OCCCCC
Mol. weight [g/mol]:	299.49

Physical Properties

Property code	Value	Unit	Source
hf	-626.87	kJ/mol	Joback Method
hvap	78.14	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	6.028		Crippen Method
mcvol	281.900	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	802.40	K	Joback Method
tc	984.56	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=U406706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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