

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

Inchi:	InChI=1S/C12H25NO2/c1-3-5-6-7-8-9-10-13-12(14)15-11-4-2/h3-11H2,1-2H3,(H,13,14)
InchiKey:	ZCMLTJOUQXELAE-UHFFFAOYSA-N
Formula:	C12H25NO2
SMILES:	CCCCCCCCN=C(O)OCCC
Mol. weight [g/mol]:	215.33

Physical Properties

Property code	Value	Unit	Source
hf	-503.03	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.688		Crippen Method
mcvol	197.360	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1824.00		NIST Webbook
tb	665.12	K	Joback Method
tc	839.33	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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