

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

Inchi:	InChI=1S/C19H39NO2/c1-3-5-7-9-10-11-12-13-14-15-17-20-19(21)22-18-16-8-6-4-2/h3-
InchiKey:	WCBALNNCJQGEQJ-UHFFFAOYSA-N
Formula:	C19H39NO2
SMILES:	CCCCCCCCCCCCN=C(O)OCCCCC
Mol. weight [g/mol]:	313.52

Physical Properties

Property code	Value	Unit	Source
hf	-647.51	kJ/mol	Joback Method
hvap	80.37	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	6.418		Crippen Method
mcvol	295.990	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinsol	2330.00		NIST Webbook
rinsol	2330.00		NIST Webbook
tb	825.28	K	Joback Method
tc	1011.08	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=U406705&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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