

Dodecanamide, N-hexadecyl-

Inchi: InChI=1S/C28H57NO/c1-3-5-7-9-11-13-14-15-16-17-19-21-23-25-27-29-28(30)26-24-22
InchiKey: OANWFRNTLIAZQA-UHFFFAOYSA-N
Formula: C28H57NO
SMILES: CCCCCCCCCCCCCCN=C(O)CCCCCCCCCCC
Mol. weight [g/mol]: 423.76

Physical Properties

Property code	Value	Unit	Source
hf	-701.05	kJ/mol	Joback Method
hvap	97.99	kJ/mol	Joback Method
log10ws	-10.53		Crippen Method
logp	10.345		Crippen Method
mcvol	416.930	ml/mol	McGowan Method
pc	652.77	kPa	Joback Method
rinpol	3263.00		NIST Webbook
rinpol	3263.00		NIST Webbook
tb	1008.78	K	Joback Method
tc	1260.92	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407578&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
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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