

Dodecanamide, N-nonyl-

Inchi: InChI=1S/C21H43NO/c1-3-5-7-9-11-12-13-15-17-19-21(23)22-20-18-16-14-10-8-6-4-2/h
InchiKey: OIQQMZIWCCNMFH-UHFFFAOYSA-N
Formula: C21H43NO
SMILES: CCCCCCCCCCCC(O)=NCCCCCCCCCC
Mol. weight [g/mol]: 325.57

Physical Properties

Property code	Value	Unit	Source
hf	-556.57	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.614		Crippen Method
mcvol	318.300	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	848.62	K	Joback Method
tc	1038.96	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407573&Units=SI>

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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