

Dodecanamide, N-heptyl-

Inchi: InChI=1S/C19H39NO/c1-3-5-7-9-10-11-12-13-15-17-19(21)20-18-16-14-8-6-4-2/h3-18H2
InchiKey: VFNYHPIRURRHIA-UHFFFAOYSA-N
Formula: C19H39NO
SMILES: CCCCCCCCCCCC(O)=NCCCCCCC
Mol. weight [g/mol]: 297.52

Physical Properties

Property code	Value	Unit	Source
hf	-515.29	kJ/mol	Joback Method
hvap	77.96	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.834		Crippen Method
mcvol	290.120	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	802.86	K	Joback Method
tc	984.91	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407571&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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