

Dodecanamide, N-3-methylbutyl-

Inchi:	InChI=1S/C17H35NO/c1-4-5-6-7-8-9-10-11-12-13-17(19)18-15-14-16(2)3/h16H,4-15H2,1
InchiKey:	ICUINMDEOUGYJX-UHFFFAOYSA-N
Formula:	C17H35NO
SMILES:	CCCCCCCCCCCC(O)=NCCC(C)C
Mol. weight [g/mol]:	269.47

Physical Properties

Property code	Value	Unit	Source
hf	-479.29	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.910		Crippen Method
mcvol	261.940	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	756.66	K	Joback Method
tc	934.77	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=U407566&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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