

Dodecanamide, N-butyl-

Other names:	N-butyl dodecanamide
Inchi:	InChI=1S/C16H33NO/c1-3-5-7-8-9-10-11-12-13-14-16(18)17-15-6-4-2/h3-15H2,1-2H3,(H
InchiKey:	NTHVNXBUGUHNAH-UHFFFAOYSA-N
Formula:	C16H33NO
SMILES:	CCCCCCCCCCCC(O)=NCCCC
Mol. weight [g/mol]:	255.44

Physical Properties

Property code	Value	Unit	Source
hf	-453.37	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.664		Crippen Method
mcvol	247.850	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		NIST Webbook
tb	734.22	K	Joback Method
tc	909.43	K	Joback Method
tf	322.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	39.00	kJ/mol	322.10	NIST Webbook

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=C6284088&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point

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