2-Naphthamide, N-butyl-

Inchi: InChI=1S/C15H17NO/c1-2-3-10-16-15(17)14-9-8-12-6-4-5-7-13(12)11-14/h4-9,11H,2-3,1

InchiKey: IKCJNZVSLPKXLB-UHFFFAOYSA-N

Formula: C15H17NO

SMILES: CCCCN=C(O)c1ccc2ccccc2c1

Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
hf	-16.60	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.944		Crippen Method
mcvol	190.540	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	761.98	K	Joback Method
tc	980.96	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407348&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