

Butanamide, N-(1-naphthyl)-

Inchi:	InChI=1S/C14H15NO/c1-2-6-14(16)15-13-10-5-8-11-7-3-4-9-12(11)13/h3-5,7-10H,2,6H2
InchiKey:	IRLQJPAKTNBBES-UHFFFAOYSA-N
Formula:	C14H15NO
SMILES:	CCCC(O)=Nc1cccc2ccccc12
Mol. weight [g/mol]:	213.28

Physical Properties

Property code	Value	Unit	Source
hf	4.04	kJ/mol	Joback Method
hvap	71.41	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.228		Crippen Method
mcvol	176.450	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	739.10	K	Joback Method
tc	961.31	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=U306920&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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