

Propanamide, N-(1-naphthyl)-3-phenyl-

Inchi: InChI=1S/C19H17NO/c21-19(14-13-15-7-2-1-3-8-15)20-18-12-6-10-16-9-4-5-11-17(16)1
InchiKey: SZEGNPOPSJJBNG-UHFFFAOYSA-N
Formula: C19H17NO
SMILES: OC(Cc1ccccc1)=Nc1cccc2ccccc12
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
hf	137.37	kJ/mol	Joback Method
hvap	84.81	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.061		Crippen Method
mcvol	223.140	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	880.18	K	Joback Method
tc	1120.97	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308122&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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