

Propanamide, 2,2,3,3,3-pentafluoro-N-1-naphthalenyl-

Other names:

Propionamide, 2,2,3,3,3-pentafluoro-N-1-naphthyl-

2,2,3,3,3-Pentafluoro-N-(1-naphthyl)propanamide

Propanamide, N-(1-naphthyl)-2,2,3,3,3-pentafluoro-

Inchi:

InChI=1S/C13H8F5NO/c14-12(15,13(16,17)18)11(20)19-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H

InchiKey:

ONHWHNOSQSZHGG-UHFFFAOYSA-N

Formula:

C13H8F5NO

SMILES:

OC(=Nc1cccc2ccccc12)C(F)(F)C(F)(F)F

Mol. weight [g/mol]:

289.20

CAS:

21970-67-2

Physical Properties

Property code	Value	Unit	Source
hf	-973.37	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.625		Crippen Method
mcpvol	171.210	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
tb	706.11	K	Joback Method
tc	909.93	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=C21970672&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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