

2-Naphthamide, N-heptyl-

Inchi:	InChI=1S/C18H23NO/c1-2-3-4-5-8-13-19-18(20)17-12-11-15-9-6-7-10-16(15)14-17/h6-7
InchiKey:	WKOCNPBMHRKZNP-UHFFFAOYSA-N
Formula:	C18H23NO
SMILES:	CCCCCCN=C(O)c1ccc2ccccc2c1
Mol. weight [g/mol]:	269.38

Physical Properties

Property code	Value	Unit	Source
hf	-78.52	kJ/mol	Joback Method
hvap	80.31	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.115		Crippen Method
mcvol	232.810	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
tb	830.62	K	Joback Method
tc	1043.17	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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