1-Naphthamide, N-butyl-N-hexyl-

Inchi: InChI=1S/C21H29NO/c1-3-5-7-10-17-22(16-6-4-2)21(23)20-15-11-13-18-12-8-9-14-19(1
InchiKey: GUWXZGNWBTXFHY-UHFFFAOYSA-N
Formula: C21H29NO
SMILES: CCCCCCN(CCCC)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
gf	317.23	kJ/mol	Joback Method
hf	-105.69	kJ/mol	Joback Method
hfus	45.44	kJ/mol	Joback Method
hvap	75.71	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	5.662		Crippen Method
mcvol	275.080	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	3039.00		NIST Webbook
rinpol	3039.00		NIST Webbook
tb	796.83	K	Joback Method
tc	1002.39	K	Joback Method
tf	480.47	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.88	J/mol×K	796.83	Joback Method
cpg	845.28	J/mol×K	831.09	Joback Method
cpg	861.63	J/mol×K	865.35	Joback Method
cpg	877.03	J/mol×K	899.61	Joback Method
cpg	891.56	J/mol×K	933.87	Joback Method
cpg	905.29	J/mol×K	968.13	Joback Method
cpg	918.33	J/mol×K	1002.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415718&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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume