

1-Naphthamide, N-butyl-N-dodecyl-

Inchi:	InChI=1S/C27H41NO/c1-3-5-7-8-9-10-11-12-13-16-23-28(22-6-4-2)27(29)26-21-17-19-2
InchiKey:	UEHGZOLSLUZTDQ-UHFFFAOYSA-N
Formula:	C27H41NO
SMILES:	CCCCCCCCCCCCN(CCCC)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	395.62

Physical Properties

Property code	Value	Unit	Source
gf	367.75	kJ/mol	Joback Method
hf	-229.53	kJ/mol	Joback Method
hfus	60.98	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	8.003		Crippen Method
mvol	359.620	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	934.11	K	Joback Method
tc	1145.28	K	Joback Method
tf	548.09	K	Joback Method
vc	1.385	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.04	J/molxK	934.11	Joback Method
cpg	1211.16	J/molxK	969.31	Joback Method
cpg	1229.24	J/molxK	1004.50	Joback Method
cpg	1246.40	J/molxK	1039.70	Joback Method
cpg	1262.75	J/molxK	1074.89	Joback Method
cpg	1278.38	J/molxK	1110.09	Joback Method
cpg	1293.42	J/molxK	1145.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415723&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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