Benzamide, N-(1-naphthyl)-4-butyl-

Inchi: InChI=1S/C21H21NO/c1-2-3-7-16-12-14-18(15-13-16)21(23)22-20-11-6-9-17-8-4-5-10-19
InchiKey: HOSGDRRMKMDTBI-UHFFFAOYSA-N
Formula: C21H21NO
SMILES: CCCCc1ccc(C(=O)Nc2cccc3ccccc23)cc1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
gf	398.62	kJ/mol	Joback Method
hf	105.31	kJ/mol	Joback Method
hfus	41.17	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.435		Crippen Method
mcvol	251.320	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	2989.00		NIST Webbook
tb	866.22	K	Joback Method
tc	1105.58	K	Joback Method
tf	539.60	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.51	J/mol×K	866.22	Joback Method
cpg	763.49	J/mol×K	906.11	Joback Method
cpg	777.40	J/mol×K	946.01	Joback Method
cpg	790.36	J/mol×K	985.90	Joback Method
cpg	802.49	J/mol×K	1025.79	Joback Method
cpg	813.92	J/mol×K	1065.68	Joback Method
cpg	824.76	J/mol×K	1105.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306998&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