Benzoic acid, 2-[(1-naphthalenylamino)carbonyl]-

Inchi: InChI=1S/C18H13NO3/c20-17(14-9-3-4-10-15(14)18(21)22)19-16-11-5-7-12-6-1-2-8-13(

InchiKey: JXTHEWSKYLZVJC-UHFFFAOYSA-N

Formula: C18H13NO3

SMILES: O=C(O)c1ccccc1C(=O)Nc1cccc2ccccc12

Mol. weight [g/mol]: 291.31

Physical Properties

Property code	Value	Unit	Source
hf	-271.16	kJ/mol	Cheméo Relay (1.0)
hfus	39.08	kJ/mol	Joback Method
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-4.01		Cheméo Relay (1.0)
logp	3.790		Crippen Method
mcvol	216.490	ml/mol	McGowan Method
tb	699.07	K	Cheméo Relay (1.0)
tf	488.36	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.23	J/mol×K	943.63	Joback Method
cpg	643.92	J/mol×K	983.72	Joback Method
cpg	652.92	J/mol×K	1023.81	Joback Method
cpg	661.35	J/mol×K	1063.90	Joback Method
cpg	669.32	J/mol×K	1103.99	Joback Method
cpg	676.93	J/mol×K	1144.08	Joback Method
cpg	684.30	J/mol×K	1184.17	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132661&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point