1-Naphthalenecarboxamide

Other names:	1-Naphthylamide
	«alpha»-Naphthamide
	1-Naphthalenecarboxamide
Inchi:	InChI=1S/C11H9NO/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H2,12,13)
InchiKey:	RMHJJUOPOWPRBP-UHFFFAOYSA-N
Formula:	C11H9NO
SMILES:	NC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	171.20

Physical Properties

Property code	Value	Unit	Source
af	0.6062		Cheméo Relay (1.0)
hf	-67.51	kJ/mol	Cheméo Relay (1.0)
hfus	21.71	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-3.06		Cheméo Relay (1.0)
logp	1.939		Crippen Method
mcvol	134.180	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	603.64	K	Cheméo Relay (1.0)
tc	900.27	K	Cheméo Relay (1.0)
tf	387.82	K	Cheméo Relay (1.0)
vc	0.488	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.65	J/mol×K	628.12	Joback Method
cpg	332.73	J/mol×K	669.96	Joback Method
cpg	343.79	J/mol×K	711.79	Joback Method
cpg	353.93	J/mol×K	753.63	Joback Method
cpg	363.22	J/mol×K	795.47	Joback Method
cpg	371.75	J/mol×K	837.30	Joback Method

cpg	379.63	J/mol×K	879.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243814&Units=SI
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):	

Legend

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