

2-Amino-N-t-butylbenzamide

Other names:	Benzamide, 2-amino-N-(1,1-dimethylethyl)- 2-Amino-N-tert-butylbenzamide
Inchi:	InChI=1S/C11H16N2O/c1-11(2,3)13-10(14)8-6-4-5-7-9(8)12/h4-7H,12H2,1-3H3,(H,13,14)
InchiKey:	YHBZJCBYHUVKCM-UHFFFAOYSA-N
Formula:	C11H16N2O
SMILES:	CC(C)(C)NC(=O)c1cccc1N
Mol. weight [g/mol]:	192.26
CAS:	1203-89-0

Physical Properties

Property code	Value	Unit	Source
gf	174.28	kJ/mol	Joback Method
hf	-79.38	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.797		Crippen Method
mvol	163.620	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	656.08	K	Joback Method
tc	888.71	K	Joback Method
tf	440.94	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.95	J/molxK	656.08	Joback Method
cpg	448.20	J/molxK	694.85	Joback Method
cpg	461.38	J/molxK	733.62	Joback Method
cpg	473.56	J/molxK	772.40	Joback Method
cpg	484.80	J/molxK	811.17	Joback Method
cpg	495.19	J/molxK	849.94	Joback Method
cpg	504.79	J/molxK	888.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C1203890&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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