butyl 4-aminobenzoate

Other names: Butamben
butyl p-aminobenzoate
Inchi: InChI=1S/C11H15NO2/c1-2-3-8-14-11(13)9-4-6-10(12)7-5-9/h4-7H,2-3,8,12H2,1H3
InchiKey: IUWVALYLNVXWKX-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 193.24
CAS: 94-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-22.95	kJ/mol	Joback Method
hf	-256.32	kJ/mol	Joback Method
hfus	25.88	kJ/mol	Joback Method
hvap	62.81	kJ/mol	Joback Method
log10ws	-3.06		Aqueous Solubility Prediction Method
log10ws	-3.13		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-3.08		Estimated Solubility Method
logp	2.226		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	631.56	K	Joback Method
tc	849.72	K	Joback Method
tf	331.00 ± 0.50	K	NIST Webbook
tf	329.00 ± 1.00	K	NIST Webbook
tf	329.00 ± 0.50	K	NIST Webbook
tf	331.00 ± 1.00	K	NIST Webbook
tf	330.98	K	Aqueous Solubility Prediction Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.64	J/mol×K	631.56	Joback Method
cpg	419.40	J/mol×K	667.92	Joback Method
cpg	432.33	J/mol×K	704.28	Joback Method
cpg	444.44	J/mol×K	740.64	Joback Method
cpg	455.75	J/mol×K	777.00	Joback Method
cpg	466.27	J/mol×K	813.36	Joback Method
cpg	476.04	J/mol×K	849.72	Joback Method
hfust	23.90	kJ/mol	330.60	NIST Webbook
hfust	20.46	kJ/mol	331.10	NIST Webbook
hfust	20.46	kJ/mol	331.10	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	1.00	NIST Webbook
tbrp	447.00	K	1.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94257&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
hfust:	Enthalpy of fusion at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume