Benzoic acid, 3-amino-, butyl ester

Inchi: InChI=1S/C11H15NO2/c1-2-3-7-14-11(13)9-5-4-6-10(12)8-9/h4-6,8H,2-3,7,12H2,1H3
InchiKey: FOFJXIVZCGTINY-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCCCOC(=O)c1cccc(N)c1
Mol. weight [g/mol]: 193.24

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	-2.60		Crippen Method
logp	2.226		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	631.56	K	Joback Method
tc	849.72	K	Joback Method
tf	408.09	K	Joback 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

Sources

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=U374539&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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