Benzoic acid, 4-amino-, pentyl ester

Other names: Amyl p-aminobenzoate
pentyl-4-aminobenzoate
Inchi: InChI=1S/C12H17NO2/c1-2-3-4-9-15-12(14)10-5-7-11(13)8-6-10/h5-8H,2-4,9,13H2,1H3
InchiKey: VKYWCHMXHQTCJQ-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CCCCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	-14.53	kJ/mol	Joback Method
hf	-276.96	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-3.26		Aqueous Solubility Prediction Method
logp	2.616		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1858.00		NIST Webbook
tb	654.44	K	Joback Method
tc	868.94	K	Joback Method
tf	419.36	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.70	J/mol×K	654.44	Joback Method
cpg	470.08	J/mol×K	690.19	Joback Method
cpg	483.58	J/mol×K	725.94	Joback Method

cpg	496.23	J/mol×K	761.69	Joback Method
cpg	508.05	J/mol×K	797.44	Joback Method
cpg	519.05	J/mol×K	833.19	Joback Method
cpg	529.27	J/mol×K	868.94	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374543&Units=SI

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

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