Benzoic acid, 3-amino-, 1-methylpropyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-25.39	kJ/mol	Joback Method
hf	-261.60	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.224		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1671.00		NIST Webbook
tb	631.12	K	Joback Method
tc	853.74	K	Joback Method
tf	393.09	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.12	J/mol×K	631.12	Joback Method
cpg	420.21	J/mol×K	668.22	Joback Method
cpg	433.41	J/mol×K	705.33	Joback Method
cpg	445.76	J/mol×K	742.43	Joback Method
cpg	457.25	J/mol×K	779.53	Joback Method
cpg	467.93	J/mol×K	816.63	Joback Method
cpg	477.80	J/mol×K	853.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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