Benzoic acid, 3-amino-, isopropyl ester

Inchi: InChI=1S/C10H13NO2/c1-7(2)13-10(12)8-4-3-5-9(11)6-8/h3-7H,11H2,1-2H3
InchiKey: OLNWTCOHKOKNJU-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CC(C)OC(=O)c1cccc(N)c1
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
gf	-33.81	kJ/mol	Joback Method
hf	-240.96	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	60.20	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.834		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	608.24	K	Joback Method
tc	835.08	K	Joback Method
tf	381.82	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.55	J/mol×K	608.24	Joback Method
cpg	370.93	J/mol×K	646.05	Joback Method
cpg	383.46	J/mol×K	683.85	Joback Method
cpg	395.16	J/mol×K	721.66	Joback Method
cpg	406.06	J/mol×K	759.47	Joback Method
cpg	416.18	J/mol×K	797.28	Joback Method
cpg	425.52	J/mol×K	835.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375455&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