Benzoic acid, 2-(isopropyl)amino-, methyl ester

Inchi: InChI=1S/C11H15NO2/c1-8(2)12-10-7-5-4-6-9(10)11(13)14-3/h4-8,12H,1-3H3
InchiKey: LXTCFGRUQWTRFS-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: COC(=O)c1ccccc1NC(C)C
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
gf	-2.45	kJ/mol	Joback Method
hf	-241.92	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.293		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
tb	608.76	K	Joback Method
tc	823.24	K	Joback Method
tf	362.49	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.17	J/mol×K	608.76	Joback Method
cpg	410.54	J/mol×K	644.51	Joback Method
cpg	424.06	J/mol×K	680.25	Joback Method
cpg	436.76	J/mol×K	716.00	Joback Method
cpg	448.64	J/mol×K	751.75	Joback Method
cpg	459.72	J/mol×K	787.50	Joback Method
cpg	470.03	J/mol×K	823.24	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=U375350&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