Benzoic acid, 3-isopropylamino-, isopropyl ester

Inchi: InChI=1S/C13H19NO2/c1-9(2)14-12-7-5-6-11(8-12)13(15)16-10(3)4/h5-10,14H,1-4H3
InchiKey: NUMSWSHSMYQMSZ-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CC(C)Nc1cccc(C(=O)OC(C)C)c1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	11.95	kJ/mol	Joback Method
hf	-288.48	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	62.29	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.072		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1700.00		NIST Webbook
tb	654.08	K	Joback Method
tc	865.76	K	Joback Method
tf	370.03	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.50	J/mol×K	654.08	Joback Method
cpg	513.34	J/mol×K	689.36	Joback Method
cpg	528.23	J/mol×K	724.64	Joback Method
cpg	542.17	J/mol×K	759.92	Joback Method
cpg	555.20	J/mol×K	795.20	Joback Method
cpg	567.33	J/mol×K	830.48	Joback Method
cpg	578.60	J/mol×K	865.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375456&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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