Benzoic acid, 3-di(isopropyl)amino-, methyl ester

Inchi: InChI=1S/C14H21NO2/c1-10(2)15(11(3)4)13-8-6-7-12(9-13)14(16)17-5/h6-11H,1-5H3
InchiKey: SJFUEBVCFPNMLM-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: COC(=O)c1cccc(N(C(C)C)C(C)C)c1
Mol. weight [g/mol]: 235.32

Physical Properties

Property code	Value	Unit	Source
gf	41.76	kJ/mol	Joback Method
hf	-295.06	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.096		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1962.00		NIST Webbook
tb	639.23	K	Joback Method
tc	845.27	K	Joback Method
tf	361.11	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.13	J/mol×K	639.23	Joback Method
cpg	550.25	J/mol×K	673.57	Joback Method
cpg	566.36	J/mol×K	707.91	Joback Method
cpg	581.48	J/mol×K	742.25	Joback Method
cpg	595.65	J/mol×K	776.59	Joback Method
cpg	608.89	J/mol×K	810.93	Joback Method
cpg	621.24	J/mol×K	845.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375342&Units=SI

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

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