Benzoic acid, 3-(dipropylamino)-, methyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	46.64	kJ/mol	Joback Method
hf	-284.50	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	60.90	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.100		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
tb	640.11	K	Joback Method
tc	838.70	K	Joback Method
tf	391.11	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.25	J/mol×K	640.11	Joback Method
cpg	548.68	J/mol×K	673.21	Joback Method
cpg	564.18	J/mol×K	706.31	Joback Method
cpg	578.78	J/mol×K	739.41	Joback Method
cpg	592.51	J/mol×K	772.51	Joback Method
cpg	605.40	J/mol×K	805.60	Joback Method
cpg	617.48	J/mol×K	838.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374485&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