Benzoic acid, 3-diethylamino-, ethyl ester

Inchi: InChI=1S/C13H19NO2/c1-4-14(5-2)12-9-7-8-11(10-12)13(15)16-6-3/h7-10H,4-6H2,1-3H
InchiKey: DASKKRDHXATCCX-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCOC(=O)c1cccc(N(CC)CC)c1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	38.22	kJ/mol	Joback Method
hf	-263.86	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.709		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
tb	617.23	K	Joback Method
tc	818.49	K	Joback Method
tf	379.84	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.53	J/mol×K	617.23	Joback Method
cpg	496.49	J/mol×K	650.77	Joback Method
cpg	511.54	J/mol×K	684.32	Joback Method
cpg	525.72	J/mol×K	717.86	Joback Method
cpg	539.05	J/mol×K	751.40	Joback Method
cpg	551.56	J/mol×K	784.95	Joback Method
cpg	563.27	J/mol×K	818.49	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=U374531&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