Benzoic acid, 4-(diethylamino)-, methyl ester

Inchi: InChI=1S/C12H17NO2/c1-4-13(5-2)11-8-6-10(7-9-11)12(14)15-3/h6-9H,4-5H2,1-3H3
InchiKey: NRZLHHHHUNKJOP-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CCN(CC)c1ccc(C(=O)OC)cc1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	29.80	kJ/mol	Joback Method
hf	-243.22	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.319		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	594.35	K	Joback Method
tc	798.55	K	Joback Method
tf	368.57	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.28	J/mol×K	594.35	Joback Method
cpg	445.68	J/mol×K	628.38	Joback Method
cpg	460.20	J/mol×K	662.42	Joback Method
cpg	473.88	J/mol×K	696.45	Joback Method
cpg	486.74	J/mol×K	730.49	Joback Method
cpg	498.79	J/mol×K	764.52	Joback Method
cpg	510.08	J/mol×K	798.55	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=U374536&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