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

Inchi: InChI=1S/C12H17NO2/c1-3-4-8-13-11-7-5-6-10(9-11)12(14)15-2/h5-7,9,13H,3-4,8H2,1-2
InchiKey: GRQYGGUSFLWQDR-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CCCCNc1cccc(C(=O)OC)c1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	8.41	kJ/mol	Joback Method
hf	-257.28	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.685		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	632.08	K	Joback Method
tc	839.02	K	Joback Method
tf	388.76	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.39	J/mol×K	632.08	Joback Method
cpg	460.06	J/mol×K	666.57	Joback Method
cpg	473.88	J/mol×K	701.06	Joback Method
cpg	486.88	J/mol×K	735.55	Joback Method
cpg	499.08	J/mol×K	770.04	Joback Method
cpg	510.49	J/mol×K	804.53	Joback Method
cpg	521.13	J/mol×K	839.02	Joback Method

Sources

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=U374487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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