Benzoic acid, 3-butylamino-, butyl ester

Inchi: InChI=1S/C15H23NO2/c1-3-5-10-16-14-9-7-8-13(12-14)15(17)18-11-6-4-2/h7-9,12,16H,3
InchiKey: VOPAHYQWXPGOEN-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: CCCCNc1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]: 249.35

Physical Properties

Property code	Value	Unit	Source
gf	33.67	kJ/mol	Joback Method
hf	-319.20	kJ/mol	Joback Method
hfus	36.14	kJ/mol	Joback Method
hvap	67.51	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.855		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	700.72	K	Joback Method
tc	899.86	K	Joback Method
tf	422.57	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.88	J/mol×K	700.72	Joback Method
cpg	618.93	J/mol×K	733.91	Joback Method
cpg	634.05	J/mol×K	767.10	Joback Method
cpg	648.26	J/mol×K	800.29	Joback Method
cpg	661.58	J/mol×K	833.48	Joback Method
cpg	674.06	J/mol×K	866.67	Joback Method
cpg	685.70	J/mol×K	899.86	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=U374540&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