Benzoic acid, 4-propylamino-, propyl ester

Inchi: InChI=1S/C13H19NO2/c1-3-9-14-12-7-5-11(6-8-12)13(15)16-10-4-2/h5-8,14H,3-4,9-10H
InchiKey: UFDQTONASDVNAF-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCCNc1ccc(C(=O)OCCC)cc1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	16.83	kJ/mol	Joback Method
hf	-277.92	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	63.06	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.075		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	654.96	K	Joback Method
tc	858.94	K	Joback Method
tf	400.03	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.54	J/mol×K	654.96	Joback Method
cpg	511.74	J/mol×K	688.96	Joback Method
cpg	526.06	J/mol×K	722.95	Joback Method
cpg	539.54	J/mol×K	756.95	Joback Method
cpg	552.17	J/mol×K	790.95	Joback Method
cpg	564.00	J/mol×K	824.95	Joback Method
cpg	575.04	J/mol×K	858.94	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=U374535&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