Benzoic acid, 2-pentylamino-, pentyl ester

Inchi: InChI=1S/C17H27NO2/c1-3-5-9-13-18-16-12-8-7-11-15(16)17(19)20-14-10-6-4-2/h7-8,11
InchiKey: WFTOPLVPNFIBQN-UHFFFAOYSA-N
Formula: C17H27NO2
SMILES: CCCCCNc1ccccc1C(=O)OCCCCC
Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
gf	50.51	kJ/mol	Joback Method
hf	-360.48	kJ/mol	Joback Method
hfus	41.32	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.636		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	746.48	K	Joback Method
tc	942.49	K	Joback Method
tf	445.11	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.05	J/mol×K	746.48	Joback Method
cpg	730.74	J/mol×K	779.15	Joback Method
cpg	746.44	J/mol×K	811.82	Joback Method
cpg	761.19	J/mol×K	844.48	Joback Method
cpg	775.02	J/mol×K	877.15	Joback Method
cpg	787.94	J/mol×K	909.82	Joback Method
cpg	800.00	J/mol×K	942.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374542&Units=SI
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

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