Propyl p-butylaminobenzoate

Inchi: InChI=1S/C14H21NO2/c1-3-5-10-15-13-8-6-12(7-9-13)14(16)17-11-4-2/h6-9,15H,3-5,10-
InchiKey: FURXDUXIEDITMM-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: CCCCNc1ccc(C(=O)OCCC)cc1
Mol. weight [g/mol]: 235.32

Physical Properties

Property code	Value	Unit	Source
gf	25.25	kJ/mol	Joback Method
hf	-298.56	kJ/mol	Joback Method
hfus	33.55	kJ/mol	Joback Method
hvap	65.29	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.465		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	677.84	K	Joback Method
tc	879.21	K	Joback Method
tf	411.30	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.06	J/mol×K	677.84	Joback Method
cpg	564.72	J/mol×K	711.40	Joback Method
cpg	579.47	J/mol×K	744.96	Joback Method
cpg	593.34	J/mol×K	778.52	Joback Method
cpg	606.36	J/mol×K	812.08	Joback Method
cpg	618.53	J/mol×K	845.65	Joback Method

cpg	629.90	J/mol×K	879.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579290&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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