P-methoxy carbanilic acid, n-pentyl ester

Inchi: InChI=1S/C13H19NO3/c1-3-4-5-10-17-13(15)14-11-6-8-12(16-2)9-7-11/h6-9H,3-5,10H2,
InchiKey: OSJQVPFGVXKNJR-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: CCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 237.29
CAS: 93759-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-88.17	kJ/mol	Joback Method
hf	-410.14	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	65.47	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.434		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
tb	677.38	K	Joback Method
tc	879.64	K	Joback Method
tf	422.26	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.25	J/mol×K	677.38	Joback Method
cpg	538.15	J/mol×K	711.09	Joback Method
cpg	552.18	J/mol×K	744.80	Joback Method
cpg	565.36	J/mol×K	778.51	Joback Method
cpg	577.70	J/mol×K	812.22	Joback Method
cpg	589.20	J/mol×K	845.93	Joback Method
cpg	599.87	J/mol×K	879.64	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=C93759923&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume