P-methoxy carbanilic acid, n-hexyl ester

Inchi: InChI=1S/C14H21NO3/c1-3-4-5-6-11-18-14(16)15-12-7-9-13(17-2)10-8-12/h7-10H,3-6,1
InchiKey: NZHRKIORKODWFQ-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 251.32
CAS: 93760-45-3

Physical Properties

Property code	Value	Unit	Source
gf	-79.75	kJ/mol	Joback Method
hf	-430.78	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	67.70	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.824		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
tb	700.26	K	Joback Method
tc	900.22	K	Joback Method
tf	433.53	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.48	J/mol×K	700.26	Joback Method
cpg	591.81	J/mol×K	733.59	Joback Method
cpg	606.24	J/mol×K	766.91	Joback Method
cpg	619.78	J/mol×K	800.24	Joback Method
cpg	632.45	J/mol×K	833.56	Joback Method
cpg	644.25	J/mol×K	866.89	Joback Method
cpg	655.19	J/mol×K	900.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93760453&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume