P-methoxy carbanilic acid, n-heptyl ester

Inchi: InChI=1S/C15H23NO3/c1-3-4-5-6-7-12-19-15(17)16-13-8-10-14(18-2)11-9-13/h8-11H,3-
InchiKey: TWIZDGKNGTYUQK-UHFFFAOYSA-N
Formula: C15H23NO3
SMILES: CCCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 265.35
CAS: 92727-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-71.33	kJ/mol	Joback Method
hf	-451.42	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.214		Crippen Method
mcvol	221.740	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
tb	723.14	K	Joback Method
tc	921.22	K	Joback Method
tf	444.80	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.94	J/mol×K	723.14	Joback Method
cpg	646.65	J/mol×K	756.15	Joback Method
cpg	661.41	J/mol×K	789.17	Joback Method
cpg	675.26	J/mol×K	822.18	Joback Method
cpg	688.20	J/mol×K	855.19	Joback Method
cpg	700.24	J/mol×K	888.21	Joback Method
cpg	711.40	J/mol×K	921.22	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=C92727156&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