P-methoxy carbanilic acid, n-undecyl ester

Inchi: InChI=1S/C19H31NO3/c1-3-4-5-6-7-8-9-10-11-16-23-19(21)20-17-12-14-18(22-2)15-13-
InchiKey: VUKNZGXNSSBZSV-UHFFFAOYSA-N
Formula: C19H31NO3
SMILES: CCCCCCCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 321.45
CAS: 95368-51-7

Physical Properties

Property code	Value	Unit	Source
gf	-37.65	kJ/mol	Joback Method
hf	-533.98	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	78.83	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.774		Crippen Method
mcvol	278.100	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
tb	814.66	K	Joback Method
tc	1010.45	K	Joback Method
tf	489.88	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.44	J/mol×K	814.66	Joback Method
cpg	876.26	J/mol×K	847.29	Joback Method
cpg	891.99	J/mol×K	879.92	Joback Method
cpg	906.65	J/mol×K	912.55	Joback Method
cpg	920.28	J/mol×K	945.18	Joback Method
cpg	932.89	J/mol×K	977.81	Joback Method
cpg	944.51	J/mol×K	1010.45	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=C95368517&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