P-methoxy carbanilic acid, n-decyl ester

Inchi: InChI=1S/C18H29NO3/c1-3-4-5-6-7-8-9-10-15-22-18(20)19-16-11-13-17(21-2)14-12-16/h
InchiKey: JNUNYCKSXQCXLL-UHFFFAOYSA-N
Formula: C18H29NO3
SMILES: CCCCCCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 307.43
CAS: 94261-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-46.07	kJ/mol	Joback Method
hf	-513.34	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	76.60	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.384		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
tb	791.78	K	Joback Method
tc	987.26	K	Joback Method
tf	478.61	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.88	J/mol×K	791.78	Joback Method
cpg	817.45	J/mol×K	824.36	Joback Method
cpg	832.98	J/mol×K	856.94	Joback Method
cpg	847.48	J/mol×K	889.52	Joback Method
cpg	860.98	J/mol×K	922.10	Joback Method
cpg	873.50	J/mol×K	954.68	Joback Method
cpg	885.05	J/mol×K	987.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94261684&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