P-methoxy carbanilic acid, n-propyl ester

Inchi: InChI=1S/C11H15NO3/c1-3-8-15-11(13)12-9-4-6-10(14-2)7-5-9/h4-7H,3,8H2,1-2H3,(H,1
InchiKey: DBQISPFSTBONKB-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: CCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 209.24
CAS: 91247-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-105.01	kJ/mol	Joback Method
hf	-368.86	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	61.02	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.654		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	631.62	K	Joback Method
tc	839.60	K	Joback Method
tf	399.72	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.86	J/mol×K	631.62	Joback Method
cpg	434.64	J/mol×K	666.28	Joback Method
cpg	447.65	J/mol×K	700.95	Joback Method
cpg	459.89	J/mol×K	735.61	Joback Method
cpg	471.36	J/mol×K	770.27	Joback Method
cpg	482.06	J/mol×K	804.93	Joback Method
cpg	492.01	J/mol×K	839.60	Joback Method

Sources

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=C91247722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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