P-methoxy carbanilic acid, methyl ester

Inchi: InChI=1S/C9H11NO3/c1-12-8-5-3-7(4-6-8)10-9(11)13-2/h3-6H,1-2H3,(H,10,11)
InchiKey: XULGIYKLMVSIEC-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: COC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 181.19
CAS: 14803-72-6

Physical Properties

Property code	Value	Unit	Source
gf	-121.85	kJ/mol	Joback Method
hf	-327.58	kJ/mol	Joback Method
hfus	21.79	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.873		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	585.86	K	Joback Method
tc	800.73	K	Joback Method
tf	377.18	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.53	J/mol×K	585.86	Joback Method
cpg	336.79	J/mol×K	621.67	Joback Method
cpg	348.38	J/mol×K	657.48	Joback Method
cpg	359.30	J/mol×K	693.29	Joback Method
cpg	369.55	J/mol×K	729.11	Joback Method
cpg	379.13	J/mol×K	764.92	Joback Method
cpg	388.03	J/mol×K	800.73	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=C14803726&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