«alpha»-Amino-3'-hydroxy-4'-methoxyacetophenc

Inchi: InChI=1S/C9H11NO3/c1-13-9-3-2-6(4-7(9)11)8(12)5-10/h2-4,11H,5,10H2,1H3
InchiKey: UHQNBTSHGKWCMC-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: COc1ccc(C(=O)CN)cc1O
Mol. weight [g/mol]: 181.19
CAS: 90765-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-194.41	kJ/mol	Joback Method
hf	-392.35	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.542		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	666.42	K	Joback Method
tc	901.76	K	Joback Method
tf	497.27	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.97	J/mol×K	666.42	Joback Method
cpg	365.65	J/mol×K	705.64	Joback Method
cpg	375.62	J/mol×K	744.87	Joback Method
cpg	384.97	J/mol×K	784.09	Joback Method
cpg	393.75	J/mol×K	823.31	Joback Method
cpg	402.03	J/mol×K	862.54	Joback Method
cpg	409.86	J/mol×K	901.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90765449&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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