2-Amino-3,5-dimethylbenzoic acid

Inchi: InChI=1S/C9H11NO2/c1-5-3-6(2)8(10)7(4-5)9(11)12/h3-4H,10H2,1-2H3,(H,11,12)
InchiKey: GIMYRAQQQBFFFJ-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: Cc1cc(C)c(N)c(C(=O)O)c1
Mol. weight [g/mol]: 165.19
CAS: 14438-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-90.87	kJ/mol	Joback Method
hf	-257.99	kJ/mol	Joback Method
hfus	22.82	kJ/mol	Joback Method
hvap	73.96	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.584		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	665.52	K	Joback Method
tc	879.01	K	Joback Method
tf	449.18	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.08	J/mol×K	665.52	Joback Method
cpg	339.74	J/mol×K	701.10	Joback Method
cpg	348.83	J/mol×K	736.68	Joback Method
cpg	357.35	J/mol×K	772.27	Joback Method
cpg	365.33	J/mol×K	807.85	Joback Method
cpg	372.78	J/mol×K	843.43	Joback Method
cpg	379.71	J/mol×K	879.01	Joback Method

Sources

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=C14438325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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