p-(aminomethyl)benzoic acid

Other names: 4-(aminomethyl)benzoic acid
Inchi: InChI=1S/C8H9NO2/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4H,5,9H2,(H,10,11)
InchiKey: QCTBMLYLENLHLA-UHFFFAOYSA-N
Formula: C8H9NO2
SMILES: NCc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 151.17

Physical Properties

Property code	Value	Unit	Source
af	0.7496		Cheméo Relay (1.0)
gf	-80.03	kJ/mol	Joback Method
hf	-308.86	kJ/mol	Cheméo Relay (1.0)
hfus	21.01	kJ/mol	Joback Method
hvap	101.07	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-1.56		Cheméo Relay (1.0)
logp	0.844		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	577.31	K	Cheméo Relay (1.0)
tc	814.17	K	Cheméo Relay (1.0)
tf	474.33	K	Cheméo Relay (1.0)
vc	0.399	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.81	J/mol×K	632.68	Joback Method
cpg	294.96	J/mol×K	668.55	Joback Method
cpg	303.51	J/mol×K	704.43	Joback Method
cpg	311.48	J/mol×K	740.30	Joback Method
cpg	318.88	J/mol×K	776.17	Joback Method
cpg	325.76	J/mol×K	812.05	Joback Method
cpg	332.13	J/mol×K	847.92	Joback Method

Sources

Cheméo Relay (1.0, beta):

Solution Thermodynamic Analysis of p-(Aminomethyl)benzoic Acid in Four Binary Solvents from 288.15 to 328.15 K:	https://www.doi.org/10.1021/acs.jced.8b00763
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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