4-AMINO-3-HYDROXYBENZOIC ACID

Inchi: InChI=1S/C7H7NO3/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3,9H,8H2,(H,10,11)
InchiKey: NFPYJDZQOKCYIE-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: Nc1ccc(C(=O)O)cc1O
Mol. weight [g/mol]: 153.14

Physical Properties

Property code	Value	Unit	Source
hf	-475.19	kJ/mol	Cheméo Relay (1.0)
hfus	24.21	kJ/mol	Joback Method
ie	8.15	eV	Cheméo Relay (1.0)
log10ws	-1.30		Cheméo Relay (1.0)
logp	0.673		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
tf	568.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.00	J/mol×K	690.42	Joback Method
cpg	283.98	J/mol×K	728.37	Joback Method
cpg	290.51	J/mol×K	766.32	Joback Method
cpg	296.65	J/mol×K	804.27	Joback Method
cpg	302.48	J/mol×K	842.23	Joback Method
cpg	308.08	J/mol×K	880.18	Joback Method
cpg	313.51	J/mol×K	918.13	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2374030&Units=SI

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

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point