3,5-diaminobenzoic acid

Inchi: InChI=1S/C7H8N2O2/c8-5-1-4(7(10)11)2-6(9)3-5/h1-3H,8-9H2,(H,10,11)
InchiKey: UENRXLSRMCSUSN-UHFFFAOYSA-N
Formula: C7H8N2O2
SMILES: Nc1cc(N)cc(C(=O)O)c1
Mol. weight [g/mol]: 152.15

Physical Properties

Property code	Value	Unit	Source
af	0.8223		Cheméo Relay (1.0)
gf	-31.63	kJ/mol	Joback Method
hf	-295.45	kJ/mol	Cheméo Relay (1.0)
hfus	23.23	kJ/mol	Joback Method
hvap	109.31	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-2.17		Cheméo Relay (1.0)
logp	0.549		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5739.21	kPa	Joback Method
tb	607.61	K	Cheméo Relay (1.0)
tc	906.57	K	Cheméo Relay (1.0)
tf	523.36	K	Cheméo Relay (1.0)
vc	0.385	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.05	J/mol×K	687.31	Joback Method
cpg	293.91	J/mol×K	725.06	Joback Method
cpg	301.21	J/mol×K	762.81	Joback Method
cpg	307.96	J/mol×K	800.56	Joback Method
cpg	314.18	J/mol×K	838.31	Joback Method
cpg	319.91	J/mol×K	876.06	Joback Method
cpg	325.16	J/mol×K	913.81	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
Solubility of 3,5-Dimethoxybenzoic Acid, 4-Cyanobenzoic Acid, 4-Acetoxybenzoic Acid, 3,5-Diaminobenzoic Acid, and 2,4-Dichlorobenzoic Acid in Ethanol:	https://www.doi.org/10.1021/je900190n
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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