3,5-Diamino-2-methylbenzoic acid

Inchi: InChI=1S/C8H10N2O2/c1-4-6(8(11)12)2-5(9)3-7(4)10/h2-3H,9-10H2,1H3,(H,11,12)
InchiKey: RKBQPUFPJRCJKE-UHFFFAOYSA-N
Formula: C8H10N2O2
SMILES: Cc1c(N)cc(N)cc1C(=O)O
Mol. weight [g/mol]: 166.18
CAS: 90007-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-32.84	kJ/mol	Joback Method
hf	-203.56	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	82.37	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	0.858		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	715.17	K	Joback Method
tc	938.54	K	Joback Method
tf	521.17	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.41	J/mol×K	715.17	Joback Method
cpg	340.98	J/mol×K	752.40	Joback Method
cpg	348.97	J/mol×K	789.63	Joback Method
cpg	356.40	J/mol×K	826.85	Joback Method
cpg	363.28	J/mol×K	864.08	Joback Method
cpg	369.63	J/mol×K	901.31	Joback Method
cpg	375.47	J/mol×K	938.54	Joback Method

Sources

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=C90007300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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