1,2-Benzenediol,4-(2-aminopropyl)-

Inchi: InChI=1S/C9H13NO2/c10-5-1-2-7-3-4-8(11)9(12)6-7/h3-4,6,11-12H,1-2,5,10H2
InchiKey: JDMNLLVJYLMTPE-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: NCCCc1ccc(O)c(O)c1
Mol. weight [g/mol]: 167.21
CAS: 555-64-6

Physical Properties

Property code	Value	Unit	Source
gf	-105.48	kJ/mol	Joback Method
hf	-313.39	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
ie	8.18 ± 0.06	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	0.989		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	5131.32	kPa	Joback Method
tb	665.77	K	Joback Method
tc	905.80	K	Joback Method
tf	524.31	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.59	J/mol×K	665.77	Joback Method
cpg	377.35	J/mol×K	705.77	Joback Method
cpg	387.45	J/mol×K	745.78	Joback Method
cpg	397.03	J/mol×K	785.78	Joback Method
cpg	406.25	J/mol×K	825.79	Joback Method
cpg	415.25	J/mol×K	865.79	Joback Method
cpg	424.20	J/mol×K	905.80	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=C555646&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
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