Alpha-resorcylamide, n-(2-aminoethyl)-

Inchi: InChI=1S/C9H12N2O3/c10-1-2-11-9(14)6-3-7(12)5-8(13)4-6/h3-5,12-13H,1-2,10H2,(H,1
InchiKey: GLIROQWIYXBHOJ-UHFFFAOYSA-N
Formula: C9H12N2O3
SMILES: NCCNC(=O)c1cc(O)cc(O)c1
Mol. weight [g/mol]: 196.20
CAS: 116465-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-145.01	kJ/mol	Joback Method
hf	-372.50	kJ/mol	Joback Method
hfus	36.57	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	-0.214		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	5739.21	kPa	Joback Method
tb	769.81	K	Joback Method
tc	1012.31	K	Joback Method
tf	626.90	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.46	J/mol×K	769.81	Joback Method
cpg	429.05	J/mol×K	810.23	Joback Method
cpg	438.27	J/mol×K	850.64	Joback Method
cpg	447.30	J/mol×K	891.06	Joback Method
cpg	456.27	J/mol×K	931.48	Joback Method
cpg	465.37	J/mol×K	971.89	Joback Method
cpg	474.73	J/mol×K	1012.31	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=C116465839&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