4-[2-(tert-butylamino)-1-hydroxyethyl]-2-(hydroxy

Inchi: InChI=1S/C13H21NO3/c1-13(2,3)14-7-12(17)9-4-5-11(16)10(6-9)8-15/h4-6,12,14-17H,7-

InchiKey: NDAUXUAQIAJITI-UHFFFAOYSA-N

Formula: C13H21NO3

SMILES: CC(C)(C)NCC(O)c1ccc(O)c(CO)c1

Mol. weight [g/mol]: 239.32

Physical Properties

Property code	Value	Unit	Source
gf	-177.11	kJ/mol	Joback Method
hf	-528.92	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	98.59	kJ/mol	Joback Method
log10ws	-0.68		Aqueous Solubility Prediction Method
logp	1.306		Crippen Method
mcvol	197.860	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	839.98	K	Joback Method
tc	1043.86	K	Joback Method
tf	427.40	K	Aqueous Solubility Prediction Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.74	J/mol×K	839.98	Joback Method
cpg	628.91	J/mol×K	873.96	Joback Method
cpg	639.63	J/mol×K	907.94	Joback Method
cpg	649.98	J/mol×K	941.92	Joback Method
cpg	660.07	J/mol×K	975.90	Joback Method
cpg	669.97	J/mol×K	1009.88	Joback Method
cpg	679.77	J/mol×K	1043.86	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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