dl-Noradrenaline

Other names:	1,2-Benzenediol, 4-(2-amino-1-hydroxyethyl)-, (.+/-.)- (.+/-.)-Noradrenaline (.+/-.)-Norepinephrine dl-Norepinephrine Benzyl alcohol, «alpha»-(aminomethyl)-3,4-dihydroxy-, (.+/-.)- DL-Arterenol 1,2-Benzenediol, 4-(2-amino-1-hydroxyethyl)- (.+/-.)-Arterenol 1,2-Benzenediol, 4-(2-amino-1-hydroxyethyl)-, (dl)- 1-(3,4-Dihydroxy)phenyl-2-aminoethanol NSC 294898 (±)-4-(2-amino-1-hydroxyethyl)pyrocatechol
Inchi:	InChI=1S/C8H11NO3/c9-4-8(12)5-1-2-6(10)7(11)3-5/h1-3,8,10-12H,4,9H2
InchiKey:	SFLSHLFXELFNJZ-UHFFFAOYSA-N
Formula:	C8H11NO3
SMILES:	NCC(O)c1ccc(O)c(O)c1
Mol. weight [g/mol]:	169.18
CAS:	138-65-8

Physical Properties

Property code	Value	Unit	Source
gf	-253.16	kJ/mol	Joback Method
hf	-450.26	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.090		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	6944.44	kPa	Joback Method
tb	734.63	K	Joback Method
tc	963.60	K	Joback Method
tf	558.86	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.93	J/mol×K	734.63	Joback Method
cpg	367.13	J/mol×K	772.79	Joback Method
cpg	374.99	J/mol×K	810.95	Joback Method
cpg	382.65	J/mol×K	849.12	Joback Method
cpg	390.25	J/mol×K	887.28	Joback Method
cpg	397.90	J/mol×K	925.44	Joback Method
cpg	405.76	J/mol×K	963.60	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C138658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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