DL-ARTERENOL

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

Physical Properties

Property code	Value	Unit	Source
hfus	27.85	kJ/mol	Joback Method
log10ws	0.14		Cheméo Relay (1.0)
logp	0.090		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
tf	468.75	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C138658&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point