Cathine

Other names:	Benzenemethanol, «alpha»-(1-aminoethyl)-, [S-(R*,R*)]-
	Norpseudoephedrine, (+)-
	threo-2-Amino-1-hydroxy-1-phenylpropane
	Katine
	psi-Norephedrine
	Nor-psi-ephedrine
	d-Nor-psi-ephedrine
	d-Norpseudoephedrine
	threo-1-Phenyl-1-hydroxy-2-aminopropane
	Pseudonorephedrine
	(+)-Norpseudoephedrine
	D-(+)-Norpseudoephedrine
	(+)-Pseudonorephedrine
	Cathin
	d-Norpseudoephedrin
	Norpseudoephedrine
Inchi:	InChI=1S/C9H13NO/c1-7(10)9(11)8-5-3-2-4-6-8/h2-7,9,11H,10H2,1H3/t7-,9+/m1/s1
InchiKey:	DLNKOYKMWOXYQA-APPZFPTMSA-N
Formula:	C9H13NO
SMILES:	CC(N)C(O)c1ccccc1
Mol. weight [g/mol]:	151.21
CAS:	492-39-7

Physical Properties

Property code	Value	Unit	Source
gf	62.06	kJ/mol	Joback Method
hf	-121.56	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.067		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	1303.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1377.00		NIST Webbook

rinpol	1303.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1310.00		NIST Webbook
ripol	2358.00		NIST Webbook
ripol	2341.00		NIST Webbook
ripol	2333.00		NIST Webbook
tb	595.83	K	Joback Method
tc	808.08	K	Joback Method
tf	331.69	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.04	J/mol×K	595.83	Joback Method
cpg	335.03	J/mol×K	631.21	Joback Method
cpg	346.24	J/mol×K	666.58	Joback Method
cpg	356.72	J/mol×K	701.96	Joback Method
cpg	366.49	J/mol×K	737.33	Joback Method
cpg	375.60	J/mol×K	772.71	Joback Method
cpg	384.09	J/mol×K	808.08	Joback Method

Sources

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

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=C492397&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume