synephrine

Other names:	(.+-.)-synephrine
	4-hydroxy-alpha-[(methylamino)methyl]-benzenemethanol
Inchi:	InChI=1S/C9H13NO2/c1-10-6-9(12)7-2-4-8(11)5-3-7/h2-5,9-12H,6H2,1H3
InchiKey:	YRCWQPVGYLYSOX-UHFFFAOYSA-N
Formula:	C9H13NO2
SMILES:	CNCC(O)c1ccc(O)cc1
Mol. weight [g/mol]:	167.21

Physical Properties

Property code	Value	Unit	Source
gf	-67.18	kJ/mol	Joback Method
hf	-273.91	kJ/mol	Joback Method
hfus	57.00	kJ/mol	Crystal structure determination and thermal behavior upon melting of p-synephrine
hfus	99.70 ± 0.10	kJ/mol	Study of phase equilibria and the physicochemical properties of selected pharmaceuticals
hvap	73.65	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.645		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	4510.35	kPa	Joback Method
tb	654.53	K	Joback Method
tc	864.38	K	Joback Method
tf	463.53 ± 0.10	K	Study of phase equilibria and the physicochemical properties of selected pharmaceuticals
tf	472.95	K	Crystal structure determination and thermal behavior upon melting of p-synephrine
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.38	J/mol×K	829.41	Joback Method
cpg	360.90	J/mol×K	654.53	Joback Method
cpg	371.37	J/mol×K	689.51	Joback Method
cpg	381.18	J/mol×K	724.48	Joback Method
cpg	390.40	J/mol×K	759.46	Joback Method
cpg	399.12	J/mol×K	794.43	Joback Method
cpg	415.28	J/mol×K	864.38	Joback Method
rhos	1256.00	kg/m3	294.00	Crystal structure determination and thermal behavior upon melting of p-synephrine

Sources

Study of phase equilibria and the physicochemical properties of selected pharmaceuticals:	https://www.doi.org/10.1016/j.fluid.2015.07.037
Crystal structure determination and thermal behavior upon melting of p-synephrine:	https://www.doi.org/10.1016/j.tca.2016.03.010
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

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
rhos:	Solid Density

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume