Pseudoephedrine

Other names:	Pseudoephedrine, (+)-
	Benzenemethanol, «alpha»-[1-(methylamino)ethyl]-, [S-(R*,R*)]-
	«psi»-Ephedrine
	«psi»-Ephedrine, (+)-
	«psi»-Ephedrin
	(+)-Pseudoephedrine
	D-«psi»-Ephedrine
	D-isoephedrine
	D-pseudoephedrine
	trans-Ephedrine
	Isoephedrine
	L-(+)-Pseudoephedrine
	Sudafed
	Pseudoephedrine, L-(+)-
	Besan
	d-psi-Ephedrine
	psi-Ephedrine
	«alpha»-((1S)-1-(Methylamino)ethyl)benzyl alcohol, («alpha»S)-
	d-psi-2-Methylamino-1-phenyl-1-propanol
	[S-(R*,R*)]-«alpha»-[1-(methylamino)ethyl]benzenemethanol
	«alpha»-[(1S)-1-(Methylamino)ethyl]benzenemethanol, («alpha»S)-
	Pseudoephedrine d-form
	(+)-(1S,2S)-Pseudoephedrine
	(+)-threo-Ephedrine
	(1S,2S)-(+)-Pseudoephedrine
	(1S,2S)-Pseudoephedrine
	L(+)-«psi»-Ephedrine
	(+) threo-2-(methylamino)-1-phenyl-1-propanol (pseudoephedrine)
Inchi:	InChI=1S/C10H15NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,10-12H,1-2H3/t8-,10-/m0/s1
InchiKey:	KWGRBVOPPLSCSI-WPRPVWTQSA-N
Formula:	C10H15NO
SMILES:	CNC(C)C(O)c1ccccc1
Mol. weight [g/mol]:	165.23
CAS:	90-82-4

Physical Properties

Property code	Value	Unit	Source

gf	93.42	kJ/mol	Joback Method
hf	-122.52	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.328		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1350.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2213.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2195.00		NIST Webbook
ripol	2185.00		NIST Webbook
tb	596.35	K	Joback Method
tc	797.42	K	Joback Method
tf	312.36	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.03	J/mol×K	596.35	Joback Method
cpg	374.04	J/mol×K	629.86	Joback Method
cpg	386.27	J/mol×K	663.37	Joback Method
cpg	397.75	J/mol×K	696.89	Joback Method
cpg	408.51	J/mol×K	730.40	Joback Method
cpg	418.60	J/mol×K	763.91	Joback Method
cpg	428.04	J/mol×K	797.42	Joback Method
hfust	31.95	kJ/mol	392.40	NIST Webbook

Sources

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=C90824&Units=SI
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
hfust: Enthalpy of fusion at a given temperature
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