(+) threo-2-(methylamino)-1-phenyl-1-propanol (pseudoephedrine)

Other names:	(+) threo-2-(methylamino)-1-phenyl-1-propanol (pseudoephedrine)
	(+)-(1S,2S)-Pseudoephedrine
	(+)-Pseudoephedrine
	(+)-threo-Ephedrine
	(1S,2S)-(+)-Pseudoephedrine
	(1S,2S)-Pseudoephedrine
	Benzenemethanol, «alpha»-[1-(methylamino)ethyl]-, [S-(R*,R*)]-
	Besan
	D-isoephedrine
	D-pseudoephedrine
	D-«psi»-Ephedrine
	Isoephedrine
	L(+)-«psi»-Ephedrine
	L-(+)-Pseudoephedrine
	Pseudoephedrine d-form
	Pseudoephedrine, (+)-
	Pseudoephedrine, L-(+)-
	Sudafed
	[S-(R*,R*)]-«alpha»-[1-(methylamino)ethyl]benzenemethanol
	d-psi-2-Methylamino-1-phenyl-1-propanol
	d-psi-Ephedrine
	psi-Ephedrine
	trans-Ephedrine
	«alpha»-((1S)-1-(Methylamino)ethyl)benzyl alcohol, («alpha»S)-
	«alpha»-[(1S)-1-(Methylamino)ethyl]benzenemethanol, («alpha»S)-
	«psi»-Ephedrin
	«psi»-Ephedrine
	«psi»-Ephedrine, (+)-
Inchi:	InChI=1S/C10H15NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,10-12H,1-2H3
InchiKey:	KWGRBVOPPLSCSI-WPRPVWTQSA-N
Formula:	C10H15NO
SMILES:	CNC(C)C(O)c1ccccc1
Mol. weight [g/mol]:	165.23
CAS:	4125-58-0

Physical Properties

Property code	Value	Unit	Source

af	0.5901		Cheméo Relay (1.0)
gf	93.42	kJ/mol	Joback Method
hf	-116.26	kJ/mol	Cheméo Relay (1.0)
hfus	17.84	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-0.06		Cheméo Relay (1.0)
logp	1.328		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	511.99	K	Cheméo Relay (1.0)
tc	744.73	K	Cheméo Relay (1.0)
tf	379.56	K	Cheméo Relay (1.0)
vc	0.510	m3/kmol	Cheméo Relay (1.0)

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	34.10	kJ/mol	391.10	NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4125580&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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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