(+)-N-Methylephedrine

Other names:	(1S,2R)-(+)-N-Methylephedrine
	Benzenemethanol, «alpha»-[1-(dimethylamino)ethyl]-, [S-(R*,S*)]-
	L-(+)-erythro-N-methylephedrine
	d-N-methylephedrine
Inchi:	InChI=1S/C11H17NO/c1-9(12(2)3)11(13)10-7-5-4-6-8-10/h4-9,11,13H,1-3H3
InchiKey:	FMCGSUUBYTWNDP-UHFFFAOYSA-N
Formula:	C11H17NO
SMILES:	CC(C(O)c1ccccc1)N(C)C
Mol. weight [g/mol]:	179.26
CAS:	42151-56-4

Physical Properties

Property code	Value	Unit	Source
gf	123.23	kJ/mol	Joback Method
hf	-129.10	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	60.30	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.670		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	581.50	K	Joback Method
tc	776.75	K	Joback Method
tf	303.44	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.20	J/mol×K	581.50	Joback Method
cpg	409.59	J/mol×K	614.04	Joback Method
cpg	423.12	J/mol×K	646.58	Joback Method
cpg	435.84	J/mol×K	679.12	Joback Method
cpg	447.78	J/mol×K	711.67	Joback Method

cpg	458.99	J/mol×K	744.21	Joback Method
cpg	469.51	J/mol×K	776.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42151564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-Liquid Equilibria of N-Methylephedrine Enantiomers and Their Mixtures in Two Chiral Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.8b01245
Solid-Liquid Equilibria of N-Methylephedrine Enantiomers and Their Mixtures in Three Chiral Solvents Distinguished by Chain Length:	https://www.doi.org/10.1021/je1007839
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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