(1S,2R)-(+)-N-METHYLEPHEDRINE

Other names: (+)-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/t9-,11-/m1/s
InchiKey: FMCGSUUBYTWNDP-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: CC(C(O)c1ccccc1)N(C)C
Mol. weight [g/mol]: 179.26

Physical Properties

Property code	Value	Unit	Source
af	0.5738		Cheméo Relay (1.0)
gf	123.23	kJ/mol	Joback Method
hf	-124.16	kJ/mol	Cheméo Relay (1.0)
hfus	18.35	kJ/mol	Joback Method
hvap	76.90	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-0.29		Cheméo Relay (1.0)
logp	1.670		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	513.36	K	Cheméo Relay (1.0)
tc	747.54	K	Cheméo Relay (1.0)
tf	360.66	K	Cheméo Relay (1.0)
vc	0.563	m3/kmol	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Cheméo Relay (1.0):	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42151564&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
Solid-Liquid Equilibria of N-Methylephedrine Enantiomers and Their Mixtures in Two Chiral Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.8b01245

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
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