Methylephedrine

Other names:	(-) 2-Dimethylamino-1-phenyl-1-propanol (methylephedrine) (-)-N-methylephedrine (1R,2S)-(-)-N-Methylephedrine (1R,2S)-2-Dimethylamino-1-phenyl-1-propanol (1RS,2RS)-2-dimethylamino-1-phenylpropan-1-ol 2-(Dimethylamino)-1-phenyl-1-propanol , (1R,2S)- Benzenemethanol, «alpha»-((1S)-1-(dimethylamino)ethyl)-, («alpha»R)- Benzenemethanol, «alpha»-[1-(dimethylamino)ethyl]-, [R-(R*,S*)]- Benzenemethanol, Â«alphaÂ»-((1S)-1-(dimethylamino)ethyl)-, (Â«alphaÂ»R)- Benzenemethanol, Â«alphaÂ»-[1-(dimethylamino)ethyl]-, [R-(R*,S*)]- L-erythro-«alpha»-[1-(Dimethylamino)ethyl]benzyl alcohol L-erythro-Â«alphaÂ»-[1-(Dimethylamino)ethyl]benzyl alcohol Methylephedrin N,N-Dimethylnorephedrine 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:	552-79-4

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
rinpol	1441.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1430.60		NIST Webbook
rinpol	1405.00		NIST Webbook

rinpol	1400.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1430.60		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2015.00		NIST Webbook
ripol	2027.00		NIST Webbook
ripol	2022.00		NIST Webbook
ripol	2015.00		NIST Webbook
ripol	2042.00		NIST Webbook
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
hfust	21.80	kJ/mol	239.00	NIST Webbook
hfust	30.56	kJ/mol	361.20	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C552794&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

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