2-Ethylamino-1-phenylpropanol

Other names: Phenylpropanolamine, N-ethyl
Ethylnorephedrin
N-Ethylnorephedrin
Inchi: InChI=1S/C11H17NO/c1-3-12-9(2)11(13)10-7-5-4-6-8-10/h4-9,11-13H,3H2,1-2H3
InchiKey: BLJJUBZZYWYZNR-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: CCNC(C)C(O)c1ccccc1
Mol. weight [g/mol]: 179.26

Physical Properties

Property code	Value	Unit	Source
gf	101.84	kJ/mol	Joback Method
hf	-143.16	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.718		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2089.00		NIST Webbook
tb	619.23	K	Joback Method
tc	817.56	K	Joback Method
tf	323.63	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.88	J/mol×K	619.23	Joback Method
cpg	423.52	J/mol×K	652.28	Joback Method
cpg	436.35	J/mol×K	685.34	Joback Method

cpg	448.41	J/mol×K	718.39	Joback Method
cpg	459.74	J/mol×K	751.45	Joback Method
cpg	470.36	J/mol×K	784.50	Joback Method
cpg	480.32	J/mol×K	817.56	Joback Method

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=U298692&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
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