ethylephedrine

Inchi: InChI=1S/C12H19NO/c1-4-13(3)10(2)12(14)11-8-6-5-7-9-11/h5-10,12,14H,4H2,1-3H3
InchiKey: IRVLBORJKFZWMI-UHFFFAOYSA-N
Formula: C12H19NO
SMILES: CCN(C)C(C)C(O)c1ccccc1
Mol. weight [g/mol]: 193.29
CAS: 1322-32-3

Physical Properties

Property code	Value	Unit	Source
gf	131.65	kJ/mol	Joback Method
hf	-149.74	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.060		Crippen Method
mcvol	172.030	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	604.38	K	Joback Method
tc	797.18	K	Joback Method
tf	314.71	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.67	J/mol×K	604.38	Joback Method
cpg	459.61	J/mol×K	636.51	Joback Method
cpg	473.68	J/mol×K	668.65	Joback Method
cpg	486.91	J/mol×K	700.78	Joback Method
cpg	499.36	J/mol×K	732.91	Joback Method
cpg	511.06	J/mol×K	765.05	Joback Method

cpg	522.05	J/mol×K	797.18	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1322323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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