[R-(R*,R*)]-«alpha»-[1-(methylamino)ethyl]benzyl alcohol

Other names: R,R(-)-Pseudoephedrine
Inchi: InChI=1S/C10H15NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,10-12H,1-2H3/t8-,10+/m1/s1
InchiKey: KWGRBVOPPLSCSI-SCZZXKLOSA-N
Formula: C10H15NO
SMILES: CNC(C)C(O)c1ccccc1
Mol. weight [g/mol]: 165.23
CAS: 321-97-1

Physical Properties

Property code	Value	Unit	Source
gf	93.42	kJ/mol	Joback Method
hf	-122.52	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.328		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1392.20		NIST Webbook
tb	596.35	K	Joback Method
tc	797.42	K	Joback Method
tf	312.36	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.03	J/mol×K	596.35	Joback Method
cpg	374.04	J/mol×K	629.86	Joback Method
cpg	386.27	J/mol×K	663.37	Joback Method
cpg	397.75	J/mol×K	696.89	Joback Method
cpg	408.51	J/mol×K	730.40	Joback Method
cpg	418.60	J/mol×K	763.91	Joback Method
cpg	428.04	J/mol×K	797.42	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=C321971&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