Isopropylhexedrine

Inchi: InChI=1S/C10H21N/c1-9(8-11-2)10-6-4-3-5-7-10/h9-11H,3-8H2,1-2H3
InchiKey: AGJJTKRYTPXPGM-UHFFFAOYSA-N
Formula: C10H21N
SMILES: CNCC(C)C1CCCCC1
Mol. weight [g/mol]: 155.28

Physical Properties

Property code	Value	Unit	Source
gf	144.72	kJ/mol	Joback Method
hf	-147.22	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.422		Crippen Method
mcvol	150.880	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1140.00		NIST Webbook
tb	497.48	K	Joback Method
tc	700.99	K	Joback Method
tf	247.50	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.48	J/mol×K	497.48	Joback Method
cpg	375.40	J/mol×K	531.40	Joback Method
cpg	394.29	J/mol×K	565.32	Joback Method
cpg	412.17	J/mol×K	599.24	Joback Method
cpg	429.08	J/mol×K	633.15	Joback Method
cpg	445.04	J/mol×K	667.07	Joback Method
cpg	460.08	J/mol×K	700.99	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=R18012&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