Propylhexedrine acetate

Other names: Propylhexedrine, AC
Inchi: InChI=1S/C12H23NO/c1-10(13(3)11(2)14)9-12-7-5-4-6-8-12/h10,12H,4-9H2,1-3H3
InchiKey: DLRVBJBEFQXHPU-UHFFFAOYSA-N
Formula: C12H23NO
SMILES: CC(=O)N(C)C(C)CC1CCCCC1
Mol. weight [g/mol]: 197.32

Physical Properties

Property code	Value	Unit	Source
gf	54.03	kJ/mol	Joback Method
hf	-287.02	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.824		Crippen Method
mcvol	180.630	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1570.00		NIST Webbook
tb	559.38	K	Joback Method
tc	762.12	K	Joback Method
tf	299.78	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.50	J/mol×K	559.38	Joback Method
cpg	483.98	J/mol×K	593.17	Joback Method
cpg	503.30	J/mol×K	626.96	Joback Method
cpg	521.51	J/mol×K	660.75	Joback Method
cpg	538.63	J/mol×K	694.54	Joback Method
cpg	554.72	J/mol×K	728.33	Joback Method
cpg	569.81	J/mol×K	762.12	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=U119961&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