Propylhexedrine, M(HO-), AC

Inchi: InChI=1S/C14H25NO3/c1-10(15(4)11(2)16)14(18-12(3)17)13-8-6-5-7-9-13/h10,13-14H,5
InchiKey: ADGGRUXJCZVDGO-UHFFFAOYSA-N
Formula: C14H25NO3
SMILES: CC(=O)OC(C1CCCCC1)C(C)N(C)C(C)=O
Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-165.49	kJ/mol	Joback Method
hf	-578.38	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.365		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	680.99	K	Joback Method
tc	886.95	K	Joback Method
tf	379.48	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.97	J/mol×K	680.99	Joback Method
cpg	647.13	J/mol×K	715.32	Joback Method
cpg	665.08	J/mol×K	749.64	Joback Method
cpg	681.85	J/mol×K	783.97	Joback Method
cpg	697.48	J/mol×K	818.30	Joback Method
cpg	711.98	J/mol×K	852.62	Joback Method
cpg	725.41	J/mol×K	886.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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