Pholedrine, 2AC

Inchi: InChI=1S/C14H19NO3/c1-10(15(4)11(2)16)9-13-5-7-14(8-6-13)18-12(3)17/h5-8,10H,9H2
InchiKey: LHRIFRWWZCLXIB-UHFFFAOYSA-N
Formula: C14H19NO3
SMILES: CC(=O)Oc1ccc(CC(C)N(C)C(C)=O)cc1
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-84.72	kJ/mol	Joback Method
hf	-402.36	kJ/mol	Joback Method
hfus	29.55	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.021		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	693.54	K	Joback Method
tc	902.41	K	Joback Method
tf	426.04	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.94	J/mol×K	693.54	Joback Method
cpg	568.13	J/mol×K	728.35	Joback Method
cpg	582.34	J/mol×K	763.16	Joback Method
cpg	595.58	J/mol×K	797.98	Joback Method
cpg	607.91	J/mol×K	832.79	Joback Method
cpg	619.33	J/mol×K	867.60	Joback Method
cpg	629.89	J/mol×K	902.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R290927&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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