1-Phenyl-2-norbornanol, acetate

Inchi: InChI=1S/C15H18O2/c1-11(16)17-14-9-12-7-8-15(14,10-12)13-5-3-2-4-6-13/h2-6,12,14H
InchiKey: RSPCTHIVCKFIDB-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: CC(=O)OC1CC2CCC1(c1ccccc1)C2
Mol. weight [g/mol]: 230.30
CAS: 71173-15-4

Physical Properties

Property code	Value	Unit	Source
gf	50.11	kJ/mol	Joback Method
hf	-226.86	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.060		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	658.89	K	Joback Method
tc	899.04	K	Joback Method
tf	409.41	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.25	J/mol×K	658.89	Joback Method
cpg	537.31	J/mol×K	698.92	Joback Method
cpg	555.18	J/mol×K	738.94	Joback Method
cpg	572.06	J/mol×K	778.97	Joback Method
cpg	588.17	J/mol×K	818.99	Joback Method
cpg	603.74	J/mol×K	859.02	Joback Method
cpg	618.98	J/mol×K	899.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71173154&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume