4(a)-Hydroxyadamantan-2-one

Inchi: InChI=1S/C10H14O2/c11-9-6-1-5-2-7(4-6)10(12)8(9)3-5/h5-9,11H,1-4H2/t5?,6?,7?,8?,9-
InchiKey: MDHZLHGRJCMNLA-XOBOAYSZSA-N
Formula: C10H14O2
SMILES: O=C1C2CC3CC(C2)C(O)C1C3
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-71.36	kJ/mol	Joback Method
hf	-368.10	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	0.982		Crippen Method
mcvol	126.620	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	603.35	K	Joback Method
tc	816.48	K	Joback Method
tf	373.32	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.98	J/mol×K	603.35	Joback Method
cpg	390.10	J/mol×K	638.87	Joback Method
cpg	405.22	J/mol×K	674.39	Joback Method
cpg	419.39	J/mol×K	709.91	Joback Method
cpg	432.69	J/mol×K	745.44	Joback Method

cpg	445.16	J/mol×K	780.96	Joback Method
cpg	456.86	J/mol×K	816.48	Joback Method

Sources

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=R583209&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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