1-Hydroxyadamantan-2-one

Inchi: InChI=1S/C10H14O2/c11-9-8-2-6-1-7(3-8)5-10(9,12)4-6/h6-8,12H,1-5H2
InchiKey: XRDNWHRYHHULRF-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: O=C1C2CC3CC(C2)CC1(O)C3
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-69.14	kJ/mol	Joback Method
hf	-332.52	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.127		Crippen Method
mcvol	126.620	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1578.00		NIST Webbook
tb	608.26	K	Joback Method
tc	829.63	K	Joback Method
tf	401.46	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.87	J/mol×K	608.26	Joback Method
cpg	385.18	J/mol×K	645.16	Joback Method
cpg	399.55	J/mol×K	682.05	Joback Method
cpg	413.13	J/mol×K	718.95	Joback Method
cpg	426.09	J/mol×K	755.84	Joback Method

cpg	438.59	J/mol×K	792.74	Joback Method
cpg	450.79	J/mol×K	829.63	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=R583150&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