2(a),4(a)-Dihydroxyadamantane

Inchi: InChI=1S/C10H16O2/c11-9-6-1-5-2-7(4-6)10(12)8(9)3-5/h5-12H,1-4H2/t5?,6?,7?,8?,9-,1
InchiKey: PBWYCJIFRBPVPW-VBDZYGTNSA-N
Formula: C10H16O2
SMILES: OC1C2CC3CC(C2)C(O)C1C3
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-93.30	kJ/mol	Joback Method
hf	-402.97	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	0.774		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	1631.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1631.00		NIST Webbook
tb	623.04	K	Joback Method
tc	811.33	K	Joback Method
tf	361.68	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	405.24	J/mol×K	623.04	Joback Method
cpg	419.41	J/mol×K	654.42	Joback Method
cpg	432.75	J/mol×K	685.80	Joback Method
cpg	445.32	J/mol×K	717.19	Joback Method
cpg	457.18	J/mol×K	748.57	Joback Method
cpg	468.39	J/mol×K	779.95	Joback Method
cpg	479.01	J/mol×K	811.33	Joback Method
dvisc	0.0095688	Pa×s	361.68	Joback Method
dvisc	0.0044001	Pa×s	405.24	Joback Method
dvisc	0.0023527	Pa×s	448.80	Joback Method
dvisc	0.0014053	Pa×s	492.36	Joback Method
dvisc	0.0009128	Pa×s	535.92	Joback Method
dvisc	0.0006326	Pa×s	579.48	Joback Method
dvisc	0.0004615	Pa×s	623.04	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=R583170&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
dvisc:	Dynamic viscosity
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