1,2-Dihydroxyadamantane

Inchi: InChI=1S/C10H16O2/c11-9-8-2-6-1-7(3-8)5-10(9,12)4-6/h6-9,11-12H,1-5H2
InchiKey: RVIZJROSQMQZCG-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: OC1C2CC3CC(C2)CC1(O)C3
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-91.08	kJ/mol	Joback Method
hf	-367.39	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	0.918		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1592.00		NIST Webbook
tb	627.95	K	Joback Method
tc	822.67	K	Joback Method
tf	389.82	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.43	J/mol×K	627.95	Joback Method
cpg	413.86	J/mol×K	660.40	Joback Method
cpg	426.54	J/mol×K	692.86	Joback Method
cpg	438.60	J/mol×K	725.31	Joback Method

cpg	450.17	J/mol×K	757.76	Joback Method
cpg	461.39	J/mol×K	790.22	Joback Method
cpg	472.39	J/mol×K	822.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583110&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