ADAMANTANDIOL-1,3

Other names: 1,3-Dihydroxyadamantane
Inchi: InChI=1S/C10H16O2/c11-9-2-7-1-8(4-9)5-10(12,3-7)6-9/h7-8,11-12H,1-6H2
InchiKey: MOLCWHCSXCKHAP-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: OC12CC3CC(C1)CC(O)(C3)C2
Mol. weight [g/mol]: 168.24

Physical Properties

Property code	Value	Unit	Source
hf	-450.53	kJ/mol	Cheméo Relay (1.0)
hfus	10.61	kJ/mol	Joback Method
hvap	81.22	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
logp	1.062		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	543.32	K	Cheméo Relay (1.0)
tc	799.21	K	Cheméo Relay (1.0)
tf	466.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.27	J/mol×K	632.86	Joback Method
cpg	407.93	J/mol×K	666.45	Joback Method
cpg	419.97	J/mol×K	700.03	Joback Method
cpg	431.59	J/mol×K	733.62	Joback Method
cpg	443.02	J/mol×K	767.20	Joback Method

cpg	454.48	J/mol×K	800.79	Joback Method
cpg	466.18	J/mol×K	834.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5001183&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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