Adamantanol

Inchi: InChI=1S/C10H16O/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9,11H,1-6H2/t7-,8+,9-,10-
InchiKey: VLLNJDMHDJRNFK-CHIWXEEVSA-N
Formula: C10H16O
SMILES: OC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	53.45	kJ/mol	Joback Method
hf	-194.82	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.948		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1146.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1661.00		NIST Webbook
tb	540.44	K	Joback Method
tc	748.34	K	Joback Method
tf	333.24	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.80	J/mol×K	540.44	Joback Method
cpg	356.31	J/mol×K	575.09	Joback Method
cpg	371.60	J/mol×K	609.74	Joback Method
cpg	385.82	J/mol×K	644.39	Joback Method
cpg	399.13	J/mol×K	679.04	Joback Method
cpg	411.71	J/mol×K	713.69	Joback Method
cpg	423.72	J/mol×K	748.34	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=R440172&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume