2-endo -Hydroxy-2-exo -methylprotoadamantane

Inchi: InChI=1S/C11H18O/c1-11(12)9-5-7-2-3-10(11)8(4-7)6-9/h7-10,12H,2-6H2,1H3/t7-,8?,9+

InchiKey: HSUOIWZDLMCXEL-BQIANYRWSA-N

Formula: C11H18O

SMILES: CC1(O)C2CC3CCC1C(C3)C2

Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	54.16	kJ/mol	Joback Method
hf	-235.80	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.194		Crippen Method
mcvol	139.140	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	558.65	K	Joback Method
tc	763.23	K	Joback Method
tf	340.27	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.42	J/mol×K	558.65	Joback Method
cpg	406.85	J/mol×K	592.75	Joback Method
cpg	423.10	J/mol×K	626.84	Joback Method
cpg	438.33	J/mol×K	660.94	Joback Method
cpg	452.69	J/mol×K	695.04	Joback Method
cpg	466.33	J/mol×K	729.14	Joback Method
cpg	479.41	J/mol×K	763.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R287179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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