3,5-Dimethyl-1-adamantanol

Other names: Tricyclo[3.3.1.13,7]decan-1-ol, 3,5-dimethyl-
Inchi: InChI=1S/C12H20O/c1-10-3-9-4-11(2,6-10)8-12(13,5-9)7-10/h9,13H,3-8H2,1-2H3
InchiKey: LBWCITVBZLTEKW-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CC12CC3CC(C)(C1)CC(O)(C3)C2
Mol. weight [g/mol]: 180.29
CAS: 707-37-9

Physical Properties

Property code	Value	Unit	Source
gf	59.31	kJ/mol	Joback Method
hf	-205.62	kJ/mol	Joback Method
hfus	5.41	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.728		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1295.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1807.00		NIST Webbook
tb	586.68	K	Joback Method
tc	804.17	K	Joback Method
tf	403.58	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.83	J/mol×K	586.68	Joback Method
cpg	451.63	J/mol×K	622.93	Joback Method
cpg	467.30	J/mol×K	659.18	Joback Method
cpg	482.20	J/mol×K	695.43	Joback Method
cpg	496.69	J/mol×K	731.67	Joback Method
cpg	511.13	J/mol×K	767.92	Joback Method
cpg	525.89	J/mol×K	804.17	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C707379&Units=SI

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