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

Physical Properties

Property code	Value	Unit	Source
hf	-377.17	kJ/mol	Cheméo Relay (1.0)
hfus	5.41	kJ/mol	Joback Method
hvap	67.95	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
logp	2.728		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1824.00		NIST Webbook
tb	521.87	K	Cheméo Relay (1.0)
tc	764.16	K	Cheméo Relay (1.0)
tf	337.56	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point