1-Adamantanol

Other names:	1-Adamantol
	1-Adamantyl alcohol
	1-Hydroxyadamantane
	Adamantan-1-ol
	Adamantol-(1)
	NSC 108837
	NSC 91633
	Tricyclo(3.3.1.1(3,7))-n-decanol
	tricyclo[3.3.1.1(3,7)]decan-1-ol
	tricyclo[3.3.1.13,7]decan-1-ol
Inchi:	InChI=1S/C10H16O/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9,11H,1-6H2
InchiKey:	VLLNJDMHDJRNFK-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	OC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	152.23
CAS:	768-95-6

Physical Properties

Property code	Value	Unit	Source
chs	-5824.00 ± 3.00	kJ/mol	NIST Webbook
gf	53.45	kJ/mol	Joback Method
hf	-311.00 ± 3.00	kJ/mol	NIST Webbook
hf	-311.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-397.00 ± 3.00	kJ/mol	NIST Webbook
hfus	12.82	kJ/mol	Joback Method
hsub	86.80 ± 0.20	kJ/mol	NIST Webbook
hsub	86.60 ± 2.50	kJ/mol	NIST Webbook
hsub	86.00	kJ/mol	NIST Webbook
hsub	87.00 ± 3.00	kJ/mol	NIST Webbook
hsub	86.70 ± 0.20	kJ/mol	NIST Webbook
hvap	60.80	kJ/mol	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.09 ± 0.05	eV	NIST Webbook
log10ws	-2.34		Crippen Method
logp	1.948		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method

rinpol	1301.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	540.44	K	Joback Method
tc	748.34	K	Joback Method
tf	554.20 ± 0.00	K	NIST Webbook
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.71	J/mol×K	713.69	Joback Method
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	423.72	J/mol×K	748.34	Joback Method
hfust	12.36	kJ/mol	552.90	NIST Webbook
hfust	2.50	kJ/mol	369.20	NIST Webbook

hvapt	74.80	kJ/mol	298.00	Evaluation of vaporization enthalpies and liquid vapor pressures of cedrol, nerolidol, and 1-adamantanol by correlation gas chromatography
sfust	6.80	J/mol×K	369.20	NIST Webbook

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=C768956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of vaporization enthalpies and liquid vapor pressures of cedrol, nerolidol, and 1-adamantanol by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2017.07.018

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
sfust:	Entropy of fusion at a given temperature

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume