1-Adamantanemethanol

Other names:	Tricyclo[3.3.1.1(3,7)-]decane-1-methanol
	1-Adamantylmethanol
	tricyclo(3.3.1.1'3,7)dec-1-ylmethanol
	Adamantane, 1-hydroxymethyl
Inchi:	InChI=1S/C11H18O/c12-7-11-4-8-1-9(5-11)3-10(2-8)6-11/h8-10,12H,1-7H2
InchiKey:	MDVGOOIANLZFCP-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	OCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	166.26
CAS:	770-71-8

Physical Properties

Property code	Value	Unit	Source
gf	61.87	kJ/mol	Joback Method
hf	-215.46	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.195		Crippen Method
mcvol	139.140	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1435.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	1990.00		NIST Webbook
tb	563.32	K	Joback Method
tc	768.03	K	Joback Method
tf	344.51	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.32	J/mol×K	563.32	Joback Method
cpg	405.27	J/mol×K	597.44	Joback Method

cpg	421.05	J/mol×K	631.56	Joback Method
cpg	435.83	J/mol×K	665.68	Joback Method
cpg	449.76	J/mol×K	699.79	Joback Method
cpg	463.00	J/mol×K	733.91	Joback Method
cpg	475.71	J/mol×K	768.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C770718&Units=SI
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

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