2-Methyl-2-adamantanol

Other names: Tricyclo(3.3.1.1(3,7))decan-2-ol, 2-methyl-
2-Adamantanol, 2-methyl-
Inchi: InChI=1S/C11H18O/c1-11(12)9-3-7-2-8(5-9)6-10(11)4-7/h7-10,12H,2-6H2,1H3
InchiKey: JKOZWMQUOWYZAB-UHFFFAOYSA-N
Formula: C11H18O
SMILES: CC1(O)C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 166.26
CAS: 702-98-7

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
hsub	91.40 ± 0.30	kJ/mol	NIST Webbook
hsub	91.30 ± 0.80	kJ/mol	NIST Webbook
hvap	54.90	kJ/mol	Joback Method
ie	9.22	eV	NIST Webbook
log10ws	-2.52		Crippen Method
logp	2.194		Crippen Method
mcvol	139.140	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1394.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1899.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1878.00		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=C702987&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
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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

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