1-Methyladamantane

Inchi: InChI=1S/C11H18/c1-11-5-8-2-9(6-11)4-10(3-8)7-11/h8-10H,2-7H2,1H3
InchiKey: UZUCFTVAWGRMTQ-UHFFFAOYSA-N
Formula: C11H18
SMILES: CC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 150.26
CAS: 768-91-2

Physical Properties

Property code	Value	Unit	Source
chs	-6663.80 ± 1.30	kJ/mol	NIST Webbook
chs	-6658.00 ± 2.00	kJ/mol	NIST Webbook
gf	198.69	kJ/mol	Joback Method
hf	-171.70 ± 2.60	kJ/mol	NIST Webbook
hf	-171.50 ± 2.90	kJ/mol	NIST Webbook
hfs	-243.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-237.30 ± 1.30	kJ/mol	NIST Webbook
hfus	11.32	kJ/mol	Joback Method
hsub	67.80 ± 1.30	kJ/mol	NIST Webbook
hsub	71.50	kJ/mol	NIST Webbook
hsub	65.60	kJ/mol	NIST Webbook
hsub	67.57	kJ/mol	NIST Webbook
hsub	68.00 ± 1.00	kJ/mol	NIST Webbook
hvap	38.53	kJ/mol	Joback Method
ie	9.24	eV	NIST Webbook
ie	9.17 ± 0.02	eV	NIST Webbook
log10ws	-3.14		Crippen Method
logp	3.223		Crippen Method
mcvol	133.270	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1162.00		NIST Webbook

rinpol	1179.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1115.30		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1171.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1313.00		NIST Webbook
tb	471.14	K	Joback Method
tc	691.15	K	Joback Method
tf	392.00 ± 3.71	K	NIST Webbook
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.64	J/mol×K	581.14	Joback Method
cpg	397.83	J/mol×K	617.81	Joback Method
cpg	413.83	J/mol×K	654.48	Joback Method

cpg	319.89	J/mol×K	471.14	Joback Method
cpg	341.86	J/mol×K	507.81	Joback Method
cpg	362.04	J/mol×K	544.48	Joback Method
cpg	428.81	J/mol×K	691.15	Joback Method
hfust	1.91	kJ/mol	169.50	NIST Webbook
hfust	3.71	kJ/mol	392.00	NIST Webbook
hfust	1.47	kJ/mol	211.50	NIST Webbook
hfust	3.71	kJ/mol	392.00	NIST Webbook
hsubt	67.60 ± 0.50	kJ/mol	321.00	NIST Webbook
sfust	9.46	J/mol×K	392.00	NIST Webbook
sfust	6.95	J/mol×K	211.50	NIST Webbook
sfust	11.27	J/mol×K	169.50	NIST Webbook

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=C768912&Units=SI

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
hsubt: Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume