1,3,5,7-Tetramethyl-adamantane

Inchi: InChI=1S/C14H24/c1-11-5-12(2)8-13(3,6-11)10-14(4,7-11)9-12/h5-10H2,1-4H3
InchiKey: UJSORZVCMMYGBS-UHFFFAOYSA-N
Formula: C14H24
SMILES: CC12CC3(C)CC(C)(C1)CC(C)(C2)C3
Mol. weight [g/mol]: 192.34
CAS: 1687-36-1

Physical Properties

Property code	Value	Unit	Source
chs	-8577.00 ± 2.00	kJ/mol	NIST Webbook
chs	-8560.00 ± 4.00	kJ/mol	NIST Webbook
gf	207.48	kJ/mol	Joback Method
hf	-284.60 ± 6.90	kJ/mol	NIST Webbook
hf	-282.10 ± 7.00	kJ/mol	NIST Webbook
hfs	-362.10 ± 1.90	kJ/mol	NIST Webbook
hfs	-379.00 ± 4.00	kJ/mol	NIST Webbook
hfus	0.20	kJ/mol	Joback Method
hsub	84.00 ± 1.00	kJ/mol	NIST Webbook
hsub	77.50	kJ/mol	NIST Webbook
hsub	81.13	kJ/mol	NIST Webbook
hsub	96.90	kJ/mol	NIST Webbook
hsub	83.70 ± 1.30	kJ/mol	NIST Webbook
hvap	41.76	kJ/mol	Joback Method
ie	9.23	eV	NIST Webbook
log10ws	-4.40		Crippen Method
logp	4.393		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1169.00		NIST Webbook

rinpol	1162.00		NIST Webbook
tb	540.50	K	Joback Method
tc	777.93	K	Joback Method
tf	337.20 ± 0.20	K	NIST Webbook
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.57	J/mol×K	698.78	Joback Method
cpg	565.47	J/mol×K	738.36	Joback Method
cpg	466.97	J/mol×K	540.50	Joback Method
cpg	489.65	J/mol×K	580.07	Joback Method
cpg	510.26	J/mol×K	619.64	Joback Method
cpg	529.37	J/mol×K	659.21	Joback Method
cpg	583.64	J/mol×K	777.93	Joback Method
hfust	0.23	kJ/mol	183.30	NIST Webbook
hfust	9.82	kJ/mol	337.20	NIST Webbook
hfust	9.82	kJ/mol	337.20	NIST Webbook
hsubt	81.00 ± 11.00	kJ/mol	305.00	NIST Webbook
sfust	29.12	J/mol×K	337.20	NIST Webbook
sfust	1.25	J/mol×K	183.30	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=C1687361&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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