Protoadamantane

Inchi: InChI=1S/C10H16/c1-2-9-5-8-3-7(1)4-10(9)6-8/h7-10H,1-6H2
InchiKey: IPOMLSMRFPLARI-UHFFFAOYSA-N
Formula: C10H16
SMILES: C1CC2CC3CC1CC2C3
Mol. weight [g/mol]: 136.23
CAS: 53130-19-1

Physical Properties

Property code	Value	Unit	Source
chs	-6070.90 ± 1.70	kJ/mol	NIST Webbook
gf	195.76	kJ/mol	Joback Method
hf	-85.90 ± 2.50	kJ/mol	NIST Webbook
hfs	-150.80 ± 1.70	kJ/mol	NIST Webbook
hfus	15.03	kJ/mol	Joback Method
hsub	64.85	kJ/mol	NIST Webbook
hsub	64.90	kJ/mol	NIST Webbook
hsub	65.60	kJ/mol	NIST Webbook
hvap	37.46	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.833		Crippen Method
mcvol	119.180	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	448.02	K	Joback Method
tc	661.62	K	Joback Method
tf	248.52	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.92	J/mol×K	661.62	Joback Method
cpg	272.54	J/mol×K	448.02	Joback Method
cpg	293.60	J/mol×K	483.62	Joback Method
cpg	313.20	J/mol×K	519.22	Joback Method

cpg	331.44	J/mol×K	554.82	Joback Method
cpg	348.41	J/mol×K	590.42	Joback Method
cpg	364.21	J/mol×K	626.02	Joback Method
dvisc	0.0011052	Pa×s	448.02	Joback Method
dvisc	0.0006121	Pa×s	248.52	Joback Method
dvisc	0.0007158	Pa×s	281.77	Joback Method
dvisc	0.0008100	Pa×s	315.02	Joback Method
dvisc	0.0008951	Pa×s	348.27	Joback Method
dvisc	0.0009721	Pa×s	381.52	Joback Method
dvisc	0.0010419	Pa×s	414.77	Joback Method
hsubt	64.90 ± 1.80	kJ/mol	322.50	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=C53130191&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume