4-Methyldiadamantane

Inchi: InChI=1S/C15H22/c1-7-9-5-11-10-2-8-3-13(11)15(7)14(4-8)12(10)6-9/h7-15H,2-6H2,1H3
InchiKey: XCSWTEQBPOHNPL-UHFFFAOYSA-N
Formula: C15H22
SMILES: CC1C2CC3C4CC5CC3C1C(C5)C4C2
Mol. weight [g/mol]: 202.34
CAS: 30545-28-9

Physical Properties

Property code	Value	Unit	Source
chs	-8786.19 ± 0.71	kJ/mol	NIST Webbook
gf	360.43	kJ/mol	Joback Method
hf	-182.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-261.50 ± 0.71	kJ/mol	NIST Webbook
hfus	31.66	kJ/mol	Joback Method
hsub	79.41	kJ/mol	NIST Webbook
hsub	79.40	kJ/mol	NIST Webbook
hvap	47.14	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.571		Crippen Method
mcvol	167.910	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
tb	553.35	K	Joback Method
tc	766.87	K	Joback Method
tf	335.07	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.96	J/mol×K	766.87	Joback Method
cpg	601.48	J/mol×K	731.28	Joback Method
cpg	582.88	J/mol×K	695.69	Joback Method
cpg	563.00	J/mol×K	660.11	Joback Method
cpg	541.68	J/mol×K	624.52	Joback Method

cpg	518.76	J/mol×K	588.94	Joback Method
cpg	494.10	J/mol×K	553.35	Joback Method
dvisc	0.0015163	Pa×s	335.07	Joback Method
dvisc	0.0171508	Pa×s	553.35	Joback Method
dvisc	0.0131972	Pa×s	516.97	Joback Method
dvisc	0.0097600	Pa×s	480.59	Joback Method
dvisc	0.0068700	Pa×s	444.21	Joback Method
dvisc	0.0045421	Pa×s	407.83	Joback Method
dvisc	0.0027692	Pa×s	371.45	Joback Method
hsubt	103.10 ± 1.00	kJ/mol	316.00	NIST Webbook

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=C30545289&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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