

1-Methyldiadamantane

Inchi:	InChI=1S/C15H22/c1-15-7-9-3-11-10-2-8(5-13(11)15)6-14(15)12(10)4-9/h8-14H,2-7H2,1
InchiKey:	NOMKXIVITNLMHM-UHFFFAOYSA-N
Formula:	C15H22
SMILES:	CC12CC3CC4C5CC(CC41)CC2C5C3
Mol. weight [g/mol]:	202.34
CAS:	26460-76-4

Physical Properties

Property code	Value	Unit	Source
chs	-8799.40 ± 3.30	kJ/mol	NIST Webbook
gf	362.65	kJ/mol	Joback Method
hf	-166.70 ± 3.60	kJ/mol	NIST Webbook
hfs	-247.40 ± 3.30	kJ/mol	NIST Webbook
hfus	24.30	kJ/mol	Joback Method
hsub	80.70	kJ/mol	NIST Webbook
hsub	80.63	kJ/mol	NIST Webbook
hvap	46.30	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.715		Crippen Method
mcvol	167.910	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
tb	558.26	K	Joback Method
tc	780.59	K	Joback Method
tf	363.21	K	Joback Method
vc	0.663	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.93	J/mol×K	558.26	Joback Method
cpg	517.05	J/mol×K	595.32	Joback Method
cpg	539.28	J/mol×K	632.37	Joback Method
cpg	559.91	J/mol×K	669.43	Joback Method
cpg	579.20	J/mol×K	706.48	Joback Method

cpg	597.44	J/mol×K	743.54	Joback Method
cpg	614.91	J/mol×K	780.59	Joback Method
hsubt	80.70 ± 0.40	kJ/mol	321.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26460764&Units=SI
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

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
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

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