3-Methyldiadamantane

Other names: 4-Methylpentacyclo[7.3.1.1.(4,12).0(2,7).0(6,11)]tetra-decane(4-methyldiamantan)
Inchi: InChI=1S/C15H22/c1-15-5-12-9-2-8-3-10(12)14(7-15)11(4-8)13(9)6-15/h8-14H,2-7H2,1H
InchiKey: QMRMNHDCVOQSGK-UHFFFAOYSA-N
Formula: C15H22
SMILES: CC12CC3C4CC5CC3C(C1)C(C5)C4C2
Mol. weight [g/mol]: 202.34
CAS: 28375-86-2

Physical Properties

Property code	Value	Unit	Source
chs	-8786.40 ± 2.00	kJ/mol	NIST Webbook
gf	362.65	kJ/mol	Joback Method
hf	-157.30 ± 2.40	kJ/mol	NIST Webbook
hfs	-260.40 ± 2.00	kJ/mol	NIST Webbook
hfus	24.30	kJ/mol	Joback Method
hsub	103.10	kJ/mol	NIST Webbook
hsub	103.10	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.44	J/mol×K	743.54	Joback Method
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	614.91	J/mol×K	780.59	Joback Method
hsubt	79.40 ± 1.30	kJ/mol	321.50	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=C28375862&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
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