1,1'-diadamantane

Other names: 1,1'-Biadamantane
Inchi: InChI=1S/C20H30/c1-13-2-15-3-14(1)8-19(7-13,9-15)20-10-16-4-17(11-20)6-18(5-16)12-
InchiKey: MPXKIFWZOQVOLN-UHFFFAOYSA-N
Formula: C20H30
SMILES: C1C2CC3CC1CC(C14CC5CC(CC(C5)C1)C4)(C2)C3
Mol. weight [g/mol]: 270.45
CAS: 3732-31-8

Physical Properties

Property code	Value	Unit	Source
gf	431.42	kJ/mol	Joback Method
hf	-41.85	kJ/mol	Joback Method
hfus	1.15	kJ/mol	Investigation of thermodynamic properties of 1,1'-biadamantane
hsub	113.80 ± 1.40	kJ/mol	NIST Webbook
hvap	57.02	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.419		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2309.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	697.12	K	Joback Method
tc	944.73	K	Joback Method
tf	455.08	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	895.23	J/mol×K	903.46	Joback Method
cpg	763.17	J/mol×K	697.12	Joback Method
cpg	790.95	J/mol×K	738.39	Joback Method
cpg	817.50	J/mol×K	779.66	Joback Method
cpg	843.36	J/mol×K	820.93	Joback Method
cpg	869.09	J/mol×K	862.20	Joback Method
cpg	922.34	J/mol×K	944.73	Joback Method
hfust	70.00 ± 10.00	kJ/mol	561.00	NIST Webbook
hsubt	109.10 ± 1.30	kJ/mol	418.00	NIST Webbook

Sources

Investigation of thermodynamic properties of 1,1'-biadamantane:	https://www.doi.org/10.1016/j.tca.2007.03.018
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=C3732318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume