2,2'-diadamantane

Other names: 2,2'-Biadamantane
Inchi: InChI=1S/C20H30/c1-11-3-15-5-12(1)6-16(4-11)19(15)20-17-7-13-2-14(9-17)10-18(20)8-
InchiKey: FFLXOPFAPWKULC-UHFFFAOYSA-N
Formula: C20H30
SMILES: C1C2CC3CC1CC(C2)C3C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 270.45
CAS: 29542-62-9

Physical Properties

Property code	Value	Unit	Source
gf	426.98	kJ/mol	Joback Method
hf	-113.01	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	58.70	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	5.131		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2165.00		NIST Webbook
tb	687.30	K	Joback Method
tc	917.69	K	Joback Method
tf	398.80	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.22	J/mol×K	687.30	Joback Method
cpg	802.29	J/mol×K	725.70	Joback Method

cpg	828.44	J/mol×K	764.10	Joback Method
cpg	852.87	J/mol×K	802.49	Joback Method
cpg	875.81	J/mol×K	840.89	Joback Method
cpg	897.48	J/mol×K	879.29	Joback Method
cpg	918.09	J/mol×K	917.69	Joback Method
dvisc	0.0086825	Pa×s	398.80	Joback Method
dvisc	0.0128929	Pa×s	446.88	Joback Method
dvisc	0.0177296	Pa×s	494.97	Joback Method
dvisc	0.0230434	Pa×s	543.05	Joback Method
dvisc	0.0286995	Pa×s	591.13	Joback Method
dvisc	0.0345827	Pa×s	639.22	Joback Method
dvisc	0.0405988	Pa×s	687.30	Joback Method

Sources

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=C29542629&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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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