1,2'-diadamantane

Inchi: InChI=1S/C20H30/c1-12-5-17-7-13(1)8-18(6-12)19(17)20-9-14-2-15(10-20)4-16(3-14)11-
InchiKey: PHYKSFKROCAKSA-RPOBMFEDSA-N
Formula: C20H30
SMILES: C1C2CC3CC1CC(C2)C3C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	429.20	kJ/mol	Joback Method
hf	-77.43	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	57.86	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.275		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2279.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	692.21	K	Joback Method
tc	930.98	K	Joback Method
tf	426.94	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.84	J/mol×K	692.21	Joback Method
cpg	796.73	J/mol×K	732.01	Joback Method
cpg	822.99	J/mol×K	771.80	Joback Method
cpg	847.99	J/mol×K	811.60	Joback Method
cpg	872.09	J/mol×K	851.39	Joback Method

cpg	895.67	J/mol×K	891.19	Joback Method
cpg	919.09	J/mol×K	930.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R417895&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

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
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

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