4,9-dimethyl-diamantane

Inchi: InChI=1S/C16H24/c1-15-3-9-12-6-16(2)7-13(9)11(5-15)14(8-16)10(12)4-15/h9-14H,3-8H
InchiKey: FAPJFURKAYGFNX-UHFFFAOYSA-N
Formula: C16H24
SMILES: CC12CC3C4CC5(C)CC3C(C1)C(C5)C4C2
Mol. weight [g/mol]: 216.36

Physical Properties

Property code	Value	Unit	Source
gf	365.58	kJ/mol	Joback Method
hf	-33.95	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	47.37	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	4.105		Crippen Method
mcvol	182.000	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1541.00		NIST Webbook
tb	581.38	K	Joback Method
tc	808.57	K	Joback Method
tf	398.38	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.75	J/mol×K	581.38	Joback Method
cpg	568.79	J/mol×K	619.24	Joback Method
cpg	591.03	J/mol×K	657.11	Joback Method
cpg	611.84	J/mol×K	694.97	Joback Method
cpg	631.64	J/mol×K	732.84	Joback Method
cpg	650.81	J/mol×K	770.70	Joback Method
cpg	669.75	J/mol×K	808.57	Joback Method

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=R514906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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