3,4-dimethyl-diamantane

Inchi: InChI=1S/C16H24/c1-8-15-11-4-9-3-10-13(11)6-16(8,2)7-14(10)12(15)5-9/h8-15H,3-7H2
InchiKey: ZIKQQLAORFXJKW-UHFFFAOYSA-N
Formula: C16H24
SMILES: CC1C2C3CC4CC5C3CC1(C)CC5C2C4
Mol. weight [g/mol]: 216.36

Physical Properties

Property code	Value	Unit	Source
gf	363.36	kJ/mol	Joback Method
hf	-69.53	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.961		Crippen Method
mcvol	182.000	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
tb	576.47	K	Joback Method
tc	794.80	K	Joback Method
tf	370.24	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.77	J/mol×K	576.47	Joback Method
cpg	571.44	J/mol×K	612.86	Joback Method
cpg	594.33	J/mol×K	649.25	Joback Method
cpg	615.72	J/mol×K	685.64	Joback Method
cpg	635.85	J/mol×K	722.02	Joback Method
cpg	654.99	J/mol×K	758.41	Joback Method
cpg	673.40	J/mol×K	794.80	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=R514882&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

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