

Decahydro-3a-methyl-6-methylene-1-(1-methylethyl)-1H-indole

Inchi:	InChI=1S/C17H26/c1-10(2)17-8-12(7-11(17)3)13-9-16(4)6-5-14(16)15(13)17/h10,12-15H
InchiKey:	RHLJKLFLGKUCP-UHFFFAOYSA-N
Formula:	C17H26
SMILES:	C=C1CC2CC1(C(C)C)C1C2CC2(C)CCC12
Mol. weight [g/mol]:	230.39

Physical Properties

Property code	Value	Unit	Source
gf	359.50	kJ/mol	Joback Method
hf	-34.25	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.661		Crippen Method
mvol	202.650	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	605.18	K	Joback Method
tc	826.61	K	Joback Method
tf	391.11	K	Joback Method
vc	0.787	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.64	J/mol×K	605.18	Joback Method
cpg	614.59	J/mol×K	642.08	Joback Method
cpg	636.09	J/mol×K	678.99	Joback Method
cpg	656.48	J/mol×K	715.89	Joback Method
cpg	676.09	J/mol×K	752.80	Joback Method
cpg	695.24	J/mol×K	789.70	Joback Method
cpg	714.27	J/mol×K	826.61	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=R577412&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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