

2,2,4a,9-Tetramethyl-1,2,3,4,4a,5,6,14b-octahydro-

Inchi:	InChI=1S/C26H30/c1-17-6-5-7-19-18(17)8-9-21-20(19)10-11-23-22(21)12-13-26(4)15-14
InchiKey:	IULDSGKUIIHKAN-UHFFFAOYSA-N
Formula:	C26H30
SMILES:	<chem>Cc1cccc2c1ccc1c3c(ccc12)C1CC(C)(C)CCC1(C)CC3</chem>
Mol. weight [g/mol]:	342.52

Physical Properties

Property code	Value	Unit	Source
gf	533.84	kJ/mol	Joback Method
hf	136.24	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	79.23	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	7.548		Crippen Method
mcvol	292.800	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	3112.27		NIST Webbook
tb	896.67	K	Joback Method
tc	1153.12	K	Joback Method
tf	597.08	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.61	J/molxK	896.67	Joback Method
cpg	992.00	J/molxK	939.41	Joback Method
cpg	1020.46	J/molxK	982.15	Joback Method
cpg	1050.52	J/molxK	1024.90	Joback Method
cpg	1082.68	J/molxK	1067.64	Joback Method
cpg	1117.46	J/molxK	1110.38	Joback Method
cpg	1155.37	J/molxK	1153.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R179692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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