

3-Ethyl-5b,8,8,11a-tetramethyl-2,3,5b,6,7,7a,8,9,10,11,11a,11b,12,13-tetradecahydro-1

Inchi:	InChI=1S/C27H40/c1-6-18-8-9-20-19(18)10-12-22-21(20)11-13-24-26(22,4)17-14-23-25(
InchiKey:	TYBHAMOKSYDYCY-UHFFFAOYSA-N
Formula:	C27H40
SMILES:	CCC1CCc2c1ccc1c2CCC2C1(C)CCC1C(C)(C)CCCC12C
Mol. weight [g/mol]:	364.61

Physical Properties

Property code	Value	Unit	Source
gf	434.79	kJ/mol	Joback Method
hf	-120.73	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.573		Crippen Method
mcvol	324.090	ml/mol	McGowan Method
pc	1222.55	kPa	Joback Method
rinsol	2951.62		NIST Webbook
tb	889.93	K	Joback Method
tc	1134.68	K	Joback Method
tf	582.45	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.79	J/molxK	889.93	Joback Method
cpg	1183.48	J/molxK	930.72	Joback Method
cpg	1218.58	J/molxK	971.51	Joback Method
cpg	1255.66	J/molxK	1012.31	Joback Method
cpg	1295.29	J/molxK	1053.10	Joback Method
cpg	1338.04	J/molxK	1093.89	Joback Method
cpg	1384.48	J/molxK	1134.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R179701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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