

4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-

Other names: 18-Norabieta-8,11,13-triene
19-norabieta-8,11,13-triene

Inchi: InChI=1S/C19H28/c1-13(2)15-7-10-18-16(12-15)8-9-17-14(3)6-5-11-19(17,18)4/h7,10,12

InchiKey: DAYLDISWSXEJLN-UHFFFAOYSA-N

Formula: C19H28

SMILES: CC(C)c1ccc2c(c1)CCC1C(C)CCCC21C

Mol. weight [g/mol]: 256.43

Physical Properties

Property code	Value	Unit	Source
gf	283.91	kJ/mol	Joback Method
hf	-99.00	kJ/mol	Joback Method
hfus	21.55	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.450		Crippen Method
mcvol	233.090	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	687.91	K	Joback Method
tc	920.50	K	Joback Method
tf	388.85	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.99	J/mol×K	687.91	Joback Method
cpg	710.61	J/mol×K	726.68	Joback Method
cpg	732.95	J/mol×K	765.44	Joback Method
cpg	754.20	J/mol×K	804.21	Joback Method
cpg	774.58	J/mol×K	842.97	Joback Method
cpg	794.29	J/mol×K	881.74	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=U197141&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
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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