

2,6,10-Pristatriene

Inchi:	InChI=1S/C19H34/c1-16(2)10-7-12-18(5)14-9-15-19(6)13-8-11-17(3)4/h10,13-14,17H,7-9
InchiKey:	FMWKTJROXZQQOG-BFGSGJLWSA-N
Formula:	C19H34
SMILES:	CC(C)=CCCC(C)=CCCC(C)=CCCC(C)C
Mol. weight [g/mol]:	262.47

Physical Properties

Property code	Value	Unit	Source
gf	321.67	kJ/mol	Joback Method
hf	-118.48	kJ/mol	Joback Method
hfus	38.12	kJ/mol	Joback Method
hvap	57.61	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.842		Crippen Method
mcvol	265.670	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	1736.00		NIST Webbook
tb	645.80	K	Joback Method
tc	828.95	K	Joback Method
tf	231.77	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.18	J/mol×K	645.80	Joback Method
cpg	740.58	J/mol×K	676.33	Joback Method
cpg	759.98	J/mol×K	706.85	Joback Method
cpg	778.44	J/mol×K	737.38	Joback Method
cpg	796.03	J/mol×K	767.90	Joback Method
cpg	812.80	J/mol×K	798.43	Joback Method
cpg	828.82	J/mol×K	828.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214527&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
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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