

2,10-Pristadiene

Inchi:	InChI=1S/C19H36/c1-16(2)10-7-12-18(5)14-9-15-19(6)13-8-11-17(3)4/h10,13,17-18H,7-9H
InchiKey:	KAMGTSLQDYCCFE-CPNJWEJPSA-N
Formula:	C19H36
SMILES:	CC(C)=CCCC(C)CCCC(C)=CCCC(C)C
Mol. weight [g/mol]:	264.49

Physical Properties

Property code	Value	Unit	Source
gf	247.56	kJ/mol	Joback Method
hf	-231.19	kJ/mol	Joback Method
hfus	35.70	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.922		Crippen Method
mcvol	269.970	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	641.32	K	Joback Method
tc	818.95	K	Joback Method
tf	235.81	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.29	J/mol×K	641.32	Joback Method
cpg	762.15	J/mol×K	670.93	Joback Method
cpg	782.02	J/mol×K	700.53	Joback Method
cpg	800.96	J/mol×K	730.14	Joback Method
cpg	819.02	J/mol×K	759.74	Joback Method
cpg	836.24	J/mol×K	789.35	Joback Method
cpg	852.68	J/mol×K	818.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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