

7-Ethyl-1,4a,7-trimethyl-tetradecahydro-phenanthrene

Inchi: InChI=1S/C19H34/c1-5-18(3)12-10-17-15(13-18)8-9-16-14(2)7-6-11-19(16,17)4/h14-17H
InchiKey: GBAYFZPSKAXPFX-UHFFFAOYSA-N
Formula: C19H34
SMILES: CCC1(C)CCC2C(CCC3C(C)CCCC32C)C1
Mol. weight [g/mol]: 262.47

Physical Properties

Property code	Value	Unit	Source
gf	196.74	kJ/mol	Joback Method
hf	-278.43	kJ/mol	Joback Method
hfus	19.49	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	6.055		Crippen Method
mcvol	245.990	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	662.16	K	Joback Method
tc	890.11	K	Joback Method
tf	375.19	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.90	J/mol×K	662.16	Joback Method
cpg	784.44	J/mol×K	700.15	Joback Method
cpg	811.55	J/mol×K	738.14	Joback Method
cpg	837.50	J/mol×K	776.14	Joback Method
cpg	862.58	J/mol×K	814.13	Joback Method
cpg	887.08	J/mol×K	852.12	Joback Method
cpg	911.29	J/mol×K	890.11	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=R490350&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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