Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-1,4a-dimethyl-8-methylene-2-vinyl-, [4aS-(4a«alpha»,4a«beta»,7«beta»,10a«beta»)]-

Other names: Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-1,4a-dimethyl-8-methylene-2-vinyl-, [4aS-(4a«alpha»,4a«beta»,7«beta»,10a«beta»)]-; (+)-2,4b-Dimethyl-8-methylene-2-vinyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydrophenanthrene

Inchi: InChI=1S/C19H28/c1-5-18(3)12-10-17-15(13-18)8-9-16-14(2)7-6-11-19(16,17)4/h5,8,16-

InchiKey: BDOVQRGWITVTSL-UHFFFAOYSA-N

Formula: C19H28

SMILES: C=CC1(C)CCC2C(=CCC3C(=C)CCCC32C)C1

Mol. weight [g/mol]: 256.43

CAS: 26549-04-2

Physical Properties

Property code	Value	Unit	Source
gf	373.41	kJ/mol	Joback Method
hf	18.23	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.671		Crippen Method
mcvol	233.090	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1942.00		NIST Webbook
tb	671.48	K	Joback Method
tc	908.81	K	Joback Method
tf	408.87	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.83	J/mol×K	671.48	Joback Method
cpg	707.68	J/mol×K	711.04	Joback Method
cpg	731.33	J/mol×K	750.59	Joback Method
cpg	754.12	J/mol×K	790.15	Joback Method
cpg	776.39	J/mol×K	829.70	Joback Method
cpg	798.46	J/mol×K	869.26	Joback Method

cpg	820.66	J/mol×K	908.81	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=C26549042&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume