1,2,3,4,4a,9,10,10a-Octahydrophenanthrene (trans)

Other names: 1,2,3,4,4a,9,10,10a-Octahydrophenanthrene, (E)-
trans-1,2,3,4,4a,9,10,10a-Octahydrophenanthrene
Inchi: InChI=1S/C14H18/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1,3,5,7,12,14H,2,4,6,8-1
InchiKey: KFGROPZLGDSAPK-OCCSQVGLSA-N
Formula: C14H18
SMILES: c1ccc2c(c1)CCC1CCCCC21
Mol. weight [g/mol]: 186.29
CAS: 20480-67-5

Physical Properties

Property code	Value	Unit	Source
gf	267.08	kJ/mol	Joback Method
hf	26.05	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	49.87	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.907		Crippen Method
mcvol	162.640	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	573.40	K	Joback Method
tc	815.14	K	Joback Method
tf	315.32	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.81	J/mol×K	573.40	Joback Method
cpg	439.72	J/mol×K	613.69	Joback Method
cpg	459.98	J/mol×K	653.98	Joback Method
cpg	478.71	J/mol×K	694.27	Joback Method
cpg	496.03	J/mol×K	734.56	Joback Method
cpg	512.05	J/mol×K	774.85	Joback Method
cpg	526.89	J/mol×K	815.14	Joback Method

dvisc	0.0023471	Pa×s	315.32	Joback Method
dvisc	0.0016004	Pa×s	358.33	Joback Method
dvisc	0.0011846	Pa×s	401.35	Joback Method
dvisc	0.0009294	Pa×s	444.36	Joback Method
dvisc	0.0007611	Pa×s	487.37	Joback Method
dvisc	0.0006438	Pa×s	530.39	Joback Method
dvisc	0.0005584	Pa×s	573.40	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=C20480675&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume