Perhydrophenanthrene, (4a«alpha», 4b«beta», 8a«alpha», 10a«beta»)-

Other names: trans,anti,trans-Perhydrophenanthrene
Inchi: InChI=1S/C14H24/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h11-14H,1-10H2/t11-,12-,
InchiKey: GNMCGMFNBARSIY-IGQOVBAYSA-N
Formula: C14H20
SMILES: C1CCC2C(C1)CCC1CCCCC12
Mol. weight [g/mol]: 188.31
CAS: 2108-89-6

Physical Properties

Property code	Value	Unit	Source
gf	181.04	kJ/mol	Joback Method
hf	-165.03	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.393		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
tb	556.62	K	Joback Method
tc	789.03	K	Joback Method
tf	283.00 ± 1.00	K	NIST Webbook
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.30	J/mol×K	789.03	Joback Method
cpg	476.02	J/mol×K	556.62	Joback Method
cpg	503.38	J/mol×K	595.35	Joback Method
cpg	528.90	J/mol×K	634.09	Joback Method
cpg	552.65	J/mol×K	672.82	Joback Method
cpg	574.73	J/mol×K	711.56	Joback Method
cpg	595.25	J/mol×K	750.29	Joback Method
dvisc	0.0006747	Pa×s	556.62	Joback Method

dvisc	0.0033535	Pa×s	279.52	Joback Method
dvisc	0.0021240	Pa×s	325.70	Joback Method
dvisc	0.0015068	Pa×s	371.89	Joback Method
dvisc	0.0011532	Pa×s	418.07	Joback Method
dvisc	0.0009308	Pa×s	464.25	Joback Method
dvisc	0.0007810	Pa×s	510.44	Joback Method
hfust	11.83	kJ/mol	283.00	NIST Webbook

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=C2108896&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
hfust:	Enthalpy of fusion at a given temperature
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

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