

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:	GNMCGMFNBARSIIY-IGQOVBAISA-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	m ³ /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	Paxs	556.62	Joback Method

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

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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