Chrysene, octadecahydro-

Other names:	D-Homo-18-norestrane
	Octadecahydrochrysene
	Perhydrochrysene
	Chrysitane
	Perhydrochrysene, # 6
	Perhydrochrysene, # 7
	Perhydrochrysene, # 4
	Perhydrochrysene, # 5
	Perhydrochrysene, # 2
	Perhydrochrysene, # 3
	Perhydrochrysene, # 1
Inchi:	InChI=1S/C18H30/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h13-18H,
InchiKey:	ZEMKTMFBYLHVNN-UHFFFAOYSA-N
Formula:	C18H30
SMILES:	C1CCC2C(C1)CCC1C3CCCCC3CCC21
Mol. weight [g/mol]:	246.43
CAS:	2090-14-4

Physical Properties

Property code	Value	Unit	Source
gf	255.66	kJ/mol	Joback Method
hf	-201.29	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.419		Crippen Method
mcvol	221.040	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	654.48	K	Joback Method
tc	892.74	K	Joback Method
tf	334.78	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.84	J/mol×K	892.74	Joback Method
cpg	822.44	J/mol×K	853.03	Joback Method
cpg	800.42	J/mol×K	813.32	Joback Method
cpg	776.64	J/mol×K	773.61	Joback Method
cpg	750.96	J/mol×K	733.90	Joback Method
cpg	723.24	J/mol×K	694.19	Joback Method
cpg	693.36	J/mol×K	654.48	Joback Method
dvisc	0.0037204	Pa×s	334.78	Joback Method
dvisc	0.0012884	Pa×s	654.48	Joback Method
dvisc	0.0014216	Pa×s	601.20	Joback Method
dvisc	0.0015990	Pa×s	547.91	Joback Method
dvisc	0.0018446	Pa×s	494.63	Joback Method
dvisc	0.0022026	Pa×s	441.35	Joback Method
dvisc	0.0027614	Pa×s	388.06	Joback Method
hvapt	82.40	kJ/mol	313.00	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2090144&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
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