Pyrene, 1,2,3,6,7,8-hexahydro-

Other names: 1,2,3,6,7,8-Hexahydropyrene
Inchi: InChI=1S/C16H16/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h7-10H,1-6H2
InchiKey: MBAIEZXRGAOPKH-UHFFFAOYSA-N
Formula: C16H16
SMILES: c1cc2c3c(ccc4c3c1CCC4)CCC2
Mol. weight [g/mol]: 208.30
CAS: 1732-13-4

Physical Properties

Property code	Value	Unit	Source
chs	-8538.80 ± 1.70	kJ/mol	NIST Webbook
gf	401.30	kJ/mol	Joback Method
hf	40.70 ± 1.80	kJ/mol	NIST Webbook
hfs	-44.10 ± 1.90	kJ/mol	NIST Webbook
hfus	20.83	kJ/mol	Joback Method
hsub	84.80	kJ/mol	NIST Webbook
hvap	58.22	kJ/mol	Joback Method
log10ws	-5.96		Aqueous Solubility Prediction Method
logp	3.817		Crippen Method
mcvol	171.360	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	339.38		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2031.10		NIST Webbook
rinpol	339.22		NIST Webbook
rinpol	342.30		NIST Webbook
rinpol	2019.00		NIST Webbook
ss	236.26	J/mol×K	NIST Webbook
tb	653.88	K	Joback Method
tc	902.59	K	Joback Method
tf	423.64	K	Joback Method
tt	407.63 ± 0.01	K	NIST Webbook
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.40	J/mol×K	902.59	Joback Method
cpg	529.01	J/mol×K	861.14	Joback Method
cpg	455.14	J/mol×K	653.88	Joback Method
cpg	472.13	J/mol×K	695.33	Joback Method
cpg	487.82	J/mol×K	736.78	Joback Method
cpg	502.41	J/mol×K	778.23	Joback Method
cpg	516.07	J/mol×K	819.68	Joback Method
cps	255.54	J/mol×K	298.15	NIST Webbook
dvisc	0.0012702	Pa×s	615.51	Joback Method
dvisc	0.0011757	Pa×s	653.88	Joback Method
dvisc	0.0023079	Pa×s	423.64	Joback Method
dvisc	0.0019684	Pa×s	462.01	Joback Method
dvisc	0.0017204	Pa×s	500.39	Joback Method
dvisc	0.0015327	Pa×s	538.76	Joback Method
dvisc	0.0013866	Pa×s	577.13	Joback Method
hfust	18.09	kJ/mol	407.70	NIST Webbook
hfust	18.09	kJ/mol	407.70	NIST Webbook
hfust	5.02	kJ/mol	377.00	NIST Webbook
hsubt	92.30	kJ/mol	397.50	NIST Webbook
hvapt	61.50	kJ/mol	600.00	NIST Webbook
hvapt	64.20	kJ/mol	560.00	NIST Webbook
hvapt	72.00	kJ/mol	440.00	NIST Webbook
hvapt	69.40	kJ/mol	480.00	NIST Webbook
hvapt	66.80	kJ/mol	520.00	NIST Webbook
sfust	44.37	J/mol×K	407.70	NIST Webbook
sfust	13.32	J/mol×K	377.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1732134&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume