Pyrene, 4,5,9,10-tetrahydro-

Other names: 4,5,9,10-Tetrahydropyrene
Inchi: InChI=1S/C16H14/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-6H,7-10H2
InchiKey: XDFUNRTWHPWCKO-UHFFFAOYSA-N
Formula: C16H14
SMILES: c1cc2c3c(c1)CCc1cccc(c1-3)CC2
Mol. weight [g/mol]: 206.28
CAS: 781-17-9

Physical Properties

Property code	Value	Unit	Source
chs	-8322.20 ± 1.20	kJ/mol	NIST Webbook
gf	431.26	kJ/mol	Joback Method
hf	90.20 ± 1.40	kJ/mol	NIST Webbook
hfs	25.20 ± 1.50	kJ/mol	NIST Webbook
hfus	22.05	kJ/mol	Joback Method
hsub	65.00	kJ/mol	NIST Webbook
hvap	58.51	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	3.551		Crippen Method
mcvol	167.060	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	325.70		NIST Webbook
rinpol	328.95		NIST Webbook
rinpol	329.11		NIST Webbook
rinpol	329.69		NIST Webbook
rinpol	328.26		NIST Webbook
rinpol	325.70		NIST Webbook
rinpol	329.69		NIST Webbook
ss	247.77	J/mol×K	NIST Webbook
tb	653.04	K	Joback Method
tc	904.17	K	Joback Method
tf	424.40	K	Joback Method
tt	412.72 ± 0.01	K	NIST Webbook
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.52	J/mol×K	904.17	Joback Method
cpg	501.01	J/mol×K	862.32	Joback Method
cpg	489.04	J/mol×K	820.46	Joback Method
cpg	476.41	J/mol×K	778.61	Joback Method
cpg	462.92	J/mol×K	736.75	Joback Method
cpg	448.37	J/mol×K	694.90	Joback Method
cpg	432.58	J/mol×K	653.04	Joback Method
cps	257.12	J/mol×K	298.15	NIST Webbook
dvisc	0.0014104	Pa×s	576.83	Joback Method
dvisc	0.0022024	Pa×s	424.40	Joback Method
dvisc	0.0012203	Pa×s	653.04	Joback Method
dvisc	0.0019167	Pa×s	462.51	Joback Method
dvisc	0.0017037	Pa×s	500.61	Joback Method
dvisc	0.0015398	Pa×s	538.72	Joback Method
dvisc	0.0013060	Pa×s	614.93	Joback Method
hfust	17.09	kJ/mol	412.80	NIST Webbook
hsubt	90.40	kJ/mol	397.50	NIST Webbook
hvapt	56.40	kJ/mol	640.00	NIST Webbook
hvapt	59.50	kJ/mol	600.00	NIST Webbook
hvapt	62.50	kJ/mol	560.00	NIST Webbook
hvapt	65.30	kJ/mol	520.00	NIST Webbook
hvapt	70.90	kJ/mol	440.00	NIST Webbook
hvapt	68.10	kJ/mol	480.00	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=C781179&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
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