1-Hydroxypyrene

Other names:	1-Pyrenol
	3-Hydroxypyrene
	Pyren-1-ol
Inchi:	InChI=1S/C16H10O/c17-14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16(12)15(10)11/h1-9,17H
InchiKey:	BIJNHUAPTJVVNQ-UHFFFAOYSA-N
Formula:	C16H10O
SMILES:	Oc1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]:	218.25
CAS:	5315-79-7

Physical Properties

Property code	Value	Unit	Source
gf	336.56	kJ/mol	Joback Method
hf	190.46	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.290		Crippen Method
mcvol	164.330	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	731.98	K	Joback Method
tc	994.80	K	Joback Method
tf	537.64	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.91	J/mol×K	731.98	Joback Method
cpg	442.30	J/mol×K	775.78	Joback Method
cpg	453.12	J/mol×K	819.59	Joback Method
cpg	463.66	J/mol×K	863.39	Joback Method
cpg	474.22	J/mol×K	907.19	Joback Method
cpg	485.09	J/mol×K	950.99	Joback Method

cpg	496.57	J/mol×K	994.80	Joback Method
dvisc	0.0006018	Pa×s	537.64	Joback Method
dvisc	0.0004366	Pa×s	570.03	Joback Method
dvisc	0.0003278	Pa×s	602.42	Joback Method
dvisc	0.0002535	Pa×s	634.81	Joback Method
dvisc	0.0002010	Pa×s	667.20	Joback Method
dvisc	0.0001628	Pa×s	699.59	Joback Method
dvisc	0.0001343	Pa×s	731.98	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5315797&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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