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]: 218.26

Physical Properties

Property code	Value	Unit	Source
hf	84.03	kJ/mol	Cheméo Relay (1.0)
hfus	30.28	kJ/mol	Joback Method
hvap	109.59	kJ/mol	Cheméo Relay (1.0)
ie	7.11	eV	Cheméo Relay (1.0)
log10ws	-4.55		Cheméo Relay (1.0)
logp	4.290		Crippen Method
mcvol	164.330	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	686.29	K	Cheméo Relay (1.0)
tc	1034.98	K	Cheméo Relay (1.0)
tf	480.00 ± 4.00	K	NIST Webbook
vc	0.622	m3/kmol	Cheméo Relay (1.0)

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
hsubt	129.00 ± 3.20	kJ/mol	381.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5315797&Units=SI

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

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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