Benzo(a)pyren-7-ol

Other names: Benzo(a)pyrene, 7-hydroxy-
7-Hydroxybenzo(a)pyrene
7-Hydroxybenz[a]pyrene
Inchi: InChI=1S/C20H12O/c21-18-6-2-5-15-16-10-9-13-4-1-3-12-7-8-14(11-17(15)18)20(16)19(
InchiKey: CNQAYISXCZTDQX-UHFFFAOYSA-N
Formula: C20H12O
SMILES: Oc1cccc2c1cc1ccc3cccc4ccc2c1c34
Mol. weight [g/mol]: 268.31
CAS: 37994-82-4

Physical Properties

Property code	Value	Unit	Source
gf	467.26	kJ/mol	Joback Method
hf	287.50	kJ/mol	Joback Method
hfus	37.27	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	5.443		Crippen Method
mcvol	201.230	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	3252.00		NIST Webbook
rinpol	3252.00		NIST Webbook
tb	847.46	K	Joback Method
tc	1115.96	K	Joback Method
tf	627.94	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.39	J/mol×K	847.46	Joback Method
cpg	577.50	J/mol×K	892.21	Joback Method
cpg	590.79	J/mol×K	936.96	Joback Method
cpg	604.63	J/mol×K	981.71	Joback Method

cpg	619.40	J/mol×K	1026.46	Joback Method
cpg	635.46	J/mol×K	1071.21	Joback Method
cpg	653.19	J/mol×K	1115.96	Joback Method
dvisc	0.0005224	Pa×s	627.94	Joback Method
dvisc	0.0003993	Pa×s	664.53	Joback Method
dvisc	0.0003139	Pa×s	701.11	Joback Method
dvisc	0.0002527	Pa×s	737.70	Joback Method
dvisc	0.0002077	Pa×s	774.29	Joback Method
dvisc	0.0001737	Pa×s	810.87	Joback Method
dvisc	0.0001476	Pa×s	847.46	Joback Method

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=C37994824&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
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

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