Cyclopenta(cd)pyrene, 3,4-dihydro-

Other names:	Cyclopentano(cd)pyrene
	3,4-Dihydrocyclopenta(cd)pyrene
	3,4-Dimethylenepyrene
	2,3-Acepyrene
Inchi:	InChI=1S/C18H12/c1-2-11-4-6-13-7-5-12-8-9-15-10-14(3-1)16(11)18(13)17(12)15/h1-7,1
InchiKey:	LEYRJZXFRUAKLV-UHFFFAOYSA-N
Formula:	C18H10
SMILES:	c1cc2ccc3ccc4c5c(cc(c1)c2c35)CC4
Mol. weight [g/mol]:	226.27
CAS:	25732-74-5

Physical Properties

Property code	Value	Unit	Source
gf	569.32	kJ/mol	Joback Method
hf	402.85	kJ/mol	Joback Method
hfus	28.06	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	4.683		Crippen Method
mcvol	175.780	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	389.84		NIST Webbook
tb	714.22	K	Joback Method
tc	969.09	K	Joback Method
tf	499.20	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.34	J/mol×K	714.22	Joback Method
cpg	476.46	J/mol×K	756.70	Joback Method
cpg	488.76	J/mol×K	799.18	Joback Method
cpg	500.51	J/mol×K	841.66	Joback Method

cpg	511.98	J/mol×K	884.13	Joback Method
cpg	523.43	J/mol×K	926.61	Joback Method
cpg	535.14	J/mol×K	969.09	Joback Method
dvisc	0.0043835	Pa×s	499.20	Joback Method
dvisc	0.0043085	Pa×s	535.04	Joback Method
dvisc	0.0042441	Pa×s	570.87	Joback Method
dvisc	0.0041880	Pa×s	606.71	Joback Method
dvisc	0.0041388	Pa×s	642.55	Joback Method
dvisc	0.0040953	Pa×s	678.38	Joback Method
dvisc	0.0040566	Pa×s	714.22	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25732745&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
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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