

1H-Cyclopenta[a]pyrene

Inchi:	InChI=1S/C19H12/c1-3-12-7-8-15-11-14-5-2-6-16(14)17-10-9-13(4-1)18(12)19(15)17/h1-
InchiKey:	ODFNBORWBZYNEN-UHFFFAOYSA-N
Formula:	C19H12
SMILES:	C1=Cc2cc3ccc4cccc5ccc(c2C1)c3c45
Mol. weight [g/mol]:	240.30
CAS:	42315-22-0

Physical Properties

Property code	Value	Unit	Source
gf	595.60	kJ/mol	Joback Method
hf	433.83	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.153		Crippen Method
mcvol	185.570	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	740.53	K	Joback Method
tc	999.94	K	Joback Method
tf	507.71	K	Joback Method
vc	0.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.08	J/molxK	740.53	Joback Method
cpg	553.80	J/molxK	956.70	Joback Method
cpg	541.90	J/molxK	913.47	Joback Method
cpg	530.06	J/molxK	870.23	Joback Method
cpg	517.99	J/molxK	827.00	Joback Method
cpg	505.43	J/molxK	783.76	Joback Method
cpg	566.02	J/molxK	999.94	Joback Method
dvisc	0.0030808	Paxs	740.53	Joback Method
dvisc	0.0031601	Paxs	701.73	Joback Method

dvisc	0.0032511	Paxs	662.92	Joback Method
dvisc	0.0033565	Paxs	624.12	Joback Method
dvisc	0.0034800	Paxs	585.32	Joback Method
dvisc	0.0036267	Paxs	546.51	Joback Method
dvisc	0.0038035	Paxs	507.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42315220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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