

Benzo(a)acephenanthrylene

Inchi:	InChI=1S/C20H12/c1-3-7-17-13(5-1)11-15-9-10-16-12-14-6-2-4-8-18(14)20(17)19(15)16
InchiKey:	BJHAQCNKMDVELG-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	<chem>C1=Cc2cc3ccccc3c3c2c1cc1ccccc13</chem>
Mol. weight [g/mol]:	252.31

Physical Properties

Property code	Value	Unit	Source
gf	621.88	kJ/mol	Joback Method
hf	464.81	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	5.630		Crippen Method
mvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	438.90		NIST Webbook
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tb	766.84	K	Joback Method
tc	1030.60	K	Joback Method
tf	516.22	K	Joback Method
vc	0.765	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.16	J/molxK	766.84	Joback Method
cpg	534.69	J/molxK	810.80	Joback Method
cpg	547.49	J/molxK	854.76	Joback Method
cpg	559.83	J/molxK	898.72	Joback Method
cpg	572.01	J/molxK	942.68	Joback Method
cpg	584.31	J/molxK	986.64	Joback Method
cpg	597.00	J/molxK	1030.60	Joback Method
dvisc	0.0032474	Paxs	516.22	Joback Method

dvisc	0.0029976	Paxs	557.99	Joback Method
dvisc	0.0027980	Paxs	599.76	Joback Method
dvisc	0.0026352	Paxs	641.53	Joback Method
dvisc	0.0025002	Paxs	683.30	Joback Method
dvisc	0.0023865	Paxs	725.07	Joback Method
dvisc	0.0022895	Paxs	766.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411595&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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