9,10[1',2']-Benzenoanthracene, 9,10-dihydro-

Other names:	9,10-benzenoanthracene, 9,10-dihydro- 9,10-o-Benzenoanthracene, 9,10-dihydro- 9,10-o-benzeno-9,10-dihydroanthracene Anthracene, 9,10-dihydro-9,10-O-benzeno- tribenzobicyclo[2.2.2]octatriene triptycene tryptycene
Inchi:	InChI=1S/C20H14/c1-2-8-14-13(7-1)19-15-9-3-5-11-17(15)20(14)18-12-6-4-10-16(18)19/
InchiKey:	NGDCLPXRKSWRPY-UHFFFAOYSA-N
Formula:	C20H14
SMILES:	c1ccc2c(c1)C1c3ccccc3C2c2ccccc21
Mol. weight [g/mol]:	254.33
CAS:	477-75-8

Physical Properties

Property code	Value	Unit	Source
chs	-10088.20 ± 1.20	kJ/mol	NIST Webbook
gf	595.76	kJ/mol	Joback Method
hf	322.00 ± 13.00	kJ/mol	NIST Webbook
hfs	217.10 ± 1.30	kJ/mol	NIST Webbook
hfus	33.18	kJ/mol	Joback Method
hsub	104.90	kJ/mol	NIST Webbook
hsub	105.00 ± 13.00	kJ/mol	NIST Webbook
hvap	68.07	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.89	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-5.52		Crippen Method
logp	4.674		Crippen Method
mcvol	199.660	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	365.02		NIST Webbook
rinpol	366.41		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	365.02		NIST Webbook

rinpol	2228.00		NIST Webbook
ss	273.97	J/mol×K	NIST Webbook
tb	748.38	K	Joback Method
tc	1008.89	K	Joback Method
tf	481.94	K	Joback Method
tt	527.18 ± 0.02	K	NIST Webbook
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.37	J/mol×K	965.47	Joback Method
cpg	557.30	J/mol×K	748.38	Joback Method
cpg	573.12	J/mol×K	791.80	Joback Method
cpg	587.86	J/mol×K	835.22	Joback Method
cpg	601.81	J/mol×K	878.64	Joback Method
cpg	615.22	J/mol×K	922.05	Joback Method
cpg	641.52	J/mol×K	1008.89	Joback Method
cps	282.67	J/mol×K	298.15	NIST Webbook
cps	283.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0031114	Pa×s	748.38	Joback Method
dvisc	0.0037563	Pa×s	481.94	Joback Method
dvisc	0.0035923	Pa×s	526.35	Joback Method
dvisc	0.0034594	Pa×s	570.75	Joback Method
dvisc	0.0033497	Pa×s	615.16	Joback Method
dvisc	0.0032575	Pa×s	659.57	Joback Method
dvisc	0.0031790	Pa×s	703.97	Joback Method
hfust	30.29	kJ/mol	527.20	NIST Webbook
hfust	30.27	kJ/mol	527.18	NIST Webbook
hfust	30.29	kJ/mol	527.20	NIST Webbook
sfust	57.43	J/mol×K	527.18	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Triptycene, 9-Phenylanthracene, 9,10-Dimethylanthracene, and 2-Methylanthracene in Pressurized Hot Water at Temperatures from 313 K to the Melting Point:	https://www.doi.org/10.1021/je700447m
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=C477758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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https://www.chemeo.com/cid/41-682-9/9-10-1-2-Benzenoanthracene-9-10-dihydro.pdf

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